



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 11:38 AM UTC

PDB ID : 6V4T / pdb_00006v4t
BMRB ID : 30503
Title : MPER-TMD of HIV-1 Env bound with the entry inhibitor S2C3
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Deposited on : 2019-11-30

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 4%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 14 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:709 (152)	1.83	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, 4, 8, 9, 11
2	1, 6, 7, 12
3	2, 13, 14
Single-model clusters	5; 10

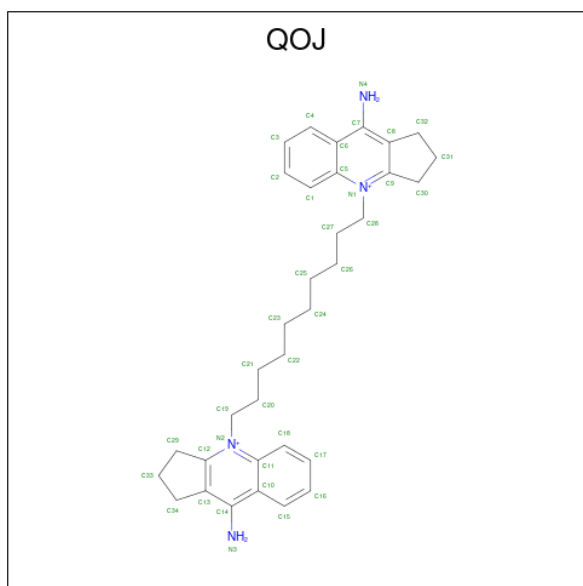
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2958 atoms, of which 1521 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	

- Molecule 2 is 4,4'-(decane-1,10-diyl)bis(9-amino-2,3-dihydro-1H-cyclopenta[b]quinolin-4-ium m) (CCD ID: QOJ) (formula: C₃₄H₄₄N₄) (labeled as "Ligand of Interest" by depositor).



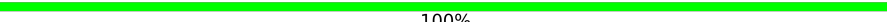
Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	N
			82	34	44	4
2	B	1	Total	C	H	N
			82	34	44	4
2	C	1	Total	C	H	N
			82	34	44	4

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:  100%

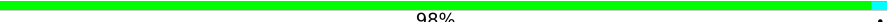
There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98%

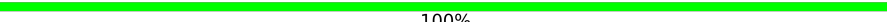


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

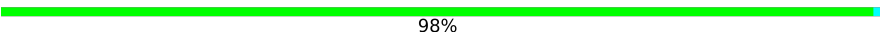
There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

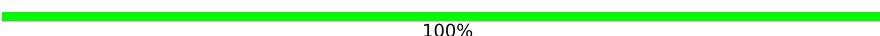
- Molecule 1: Envelope glycoprotein gp160

Chain C:  98% .



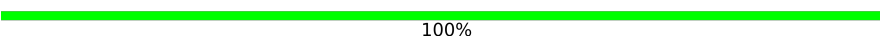
4.2.2 Score per residue for model 2

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

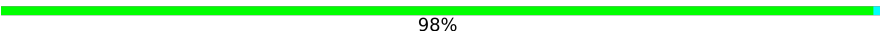
There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

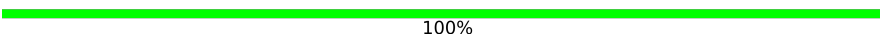
- Molecule 1: Envelope glycoprotein gp160

Chain C:  98% .



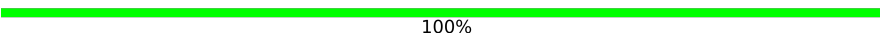
4.2.3 Score per residue for model 3

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

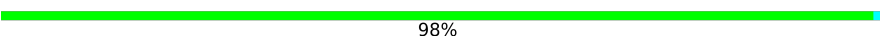
There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98% .



4.2.4 Score per residue for model 4

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98%



4.2.5 Score per residue for model 5

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98%



4.2.6 Score per residue for model 6

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98%



4.2.7 Score per residue for model 7

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98%



4.2.8 Score per residue for model 8

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98% .



4.2.9 Score per residue for model 9

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

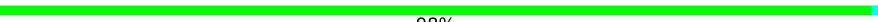
There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98% .



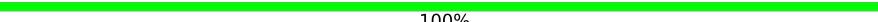
4.2.10 Score per residue for model 10

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

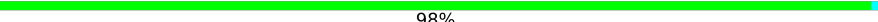
There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98% .



4.2.11 Score per residue for model 11

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98%



4.2.12 Score per residue for model 12

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98%



4.2.13 Score per residue for model 13

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98% .



4.2.14 Score per residue for model 14

- Molecule 1: Envelope glycoprotein gp160

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98% .



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 14 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	96
Number of shifts mapped to atoms	96
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

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

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

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 4% for the well-defined parts and 4% 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	96
Number of shifts mapped to atoms	96
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	48	1.55 ± 0.88	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 4%, i.e. 96 atoms were assigned a chemical shift out of a possible 2409. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	96/766 (13%)	48/310 (15%)	0/304 (0%)	48/152 (32%)
Sidechain	0/1346 (0%)	0/894 (0%)	0/402 (0%)	0/50 (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	96/2409 (4%)	48/1351 (4%)	0/841 (0%)	48/217 (22%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 96 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	96/771 (12%)	48/312 (15%)	0/306 (0%)	48/153 (31%)
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	96/2424 (4%)	48/1359 (4%)	0/846 (0%)	48/219 (22%)

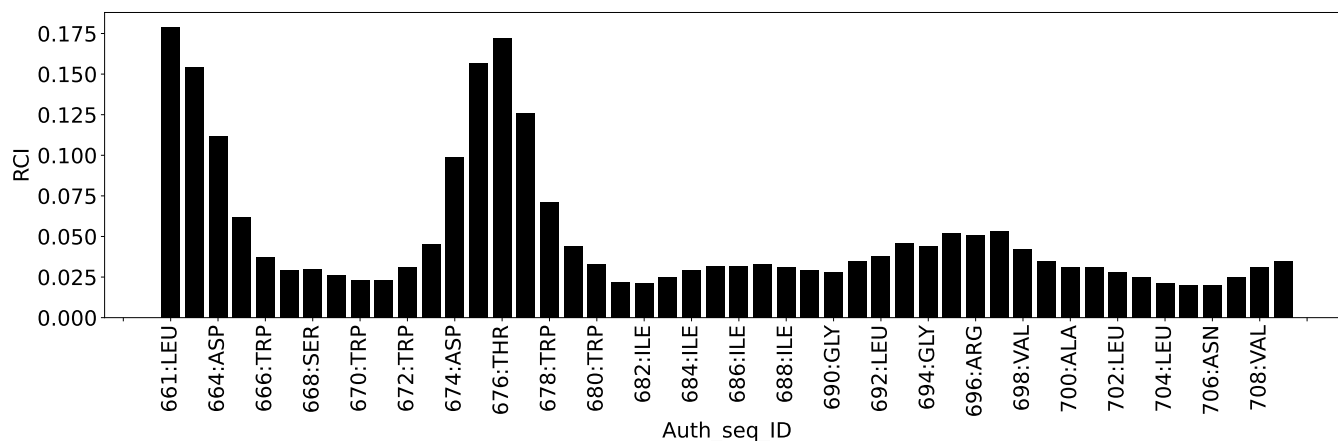
7.1.4 Statistically unusual chemical shifts [i](#)

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	669
Intra-residue ($ i-j =0$)	83
Sequential ($ i-j =1$)	288
Medium range ($ i-j >1$ and $ i-j <5$)	267
Long range ($ i-j \geq 5$)	25
Inter-chain	6
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	84
Number of unmapped restraints	0
Number of restraints per residue	4.8
Number of long range restraints per residue ¹	0.2

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	39.2	0.2
0.2-0.5 (Medium)	29.3	0.5
>0.5 (Large)	31.3	27.53

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)	7.9	4.01
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

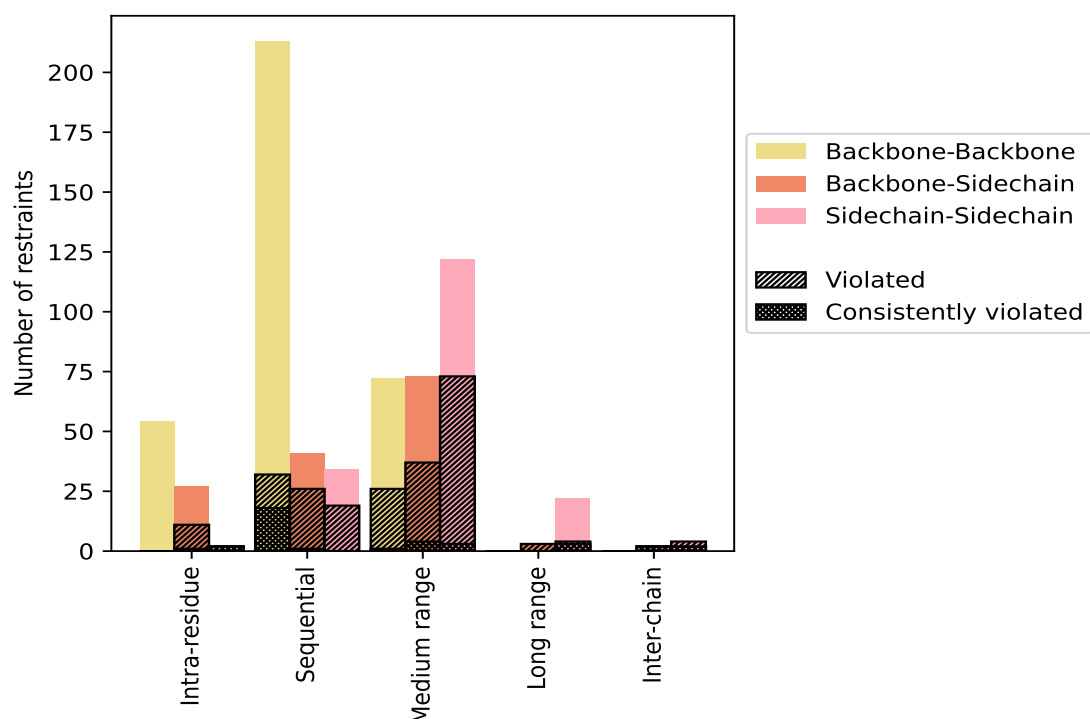
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	83	12.4	13	15.7	1.9	3	3.6	0.4
Backbone-Backbone	54	8.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	27	4.0	11	40.7	1.6	1	3.7	0.1
Sidechain-Sidechain	2	0.3	2	100.0	0.3	2	100.0	0.3
Sequential ($i-j =1$)	288	43.0	77	26.7	11.5	19	6.6	2.8
Backbone-Backbone	213	31.8	32	15.0	4.8	18	8.5	2.7
Backbone-Sidechain	41	6.1	26	63.4	3.9	1	2.4	0.1
Sidechain-Sidechain	34	5.1	19	55.9	2.8	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	267	39.9	136	50.9	20.3	8	3.0	1.2
Backbone-Backbone	72	10.8	26	36.1	3.9	1	1.4	0.1
Backbone-Sidechain	73	10.9	37	50.7	5.5	4	5.5	0.6
Sidechain-Sidechain	122	18.2	73	59.8	10.9	3	2.5	0.4
Long range ($i-j \geq 5$)	25	3.7	7	28.0	1.0	3	12.0	0.4
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	22	3.3	4	18.2	0.6	3	13.6	0.4
Inter-chain	6	0.9	6	100.0	0.9	4	66.7	0.6
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	0.3	2	100.0	0.3	2	100.0	0.3
Sidechain-Sidechain	4	0.6	4	100.0	0.6	2	50.0	0.3
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	669	100.0	239	35.7	35.7	37	5.5	5.5
Backbone-Backbone	339	50.7	58	17.1	8.7	19	5.6	2.8
Backbone-Sidechain	146	21.8	79	54.1	11.8	8	5.5	1.2
Sidechain-Sidechain	184	27.5	102	55.4	15.2	10	5.4	1.5

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	4	41	41	4	4	94	1.3	24.54	3.79	0.25
2	9	34	43	4	5	95	1.35	21.48	3.52	0.23
3	4	47	41	4	4	100	1.19	22.03	3.31	0.3
4	8	37	49	4	5	103	1.18	20.42	3.15	0.27
5	6	44	47	4	5	106	1.19	24.63	3.48	0.25
6	10	44	47	4	5	110	1.07	18.2	2.83	0.24
7	7	34	43	4	5	93	1.42	26.6	4.08	0.2
8	10	41	50	4	5	110	1.12	25.21	3.4	0.21
9	4	43	47	4	5	103	1.29	27.01	3.86	0.23
10	4	39	37	4	5	89	1.46	24.66	3.81	0.26

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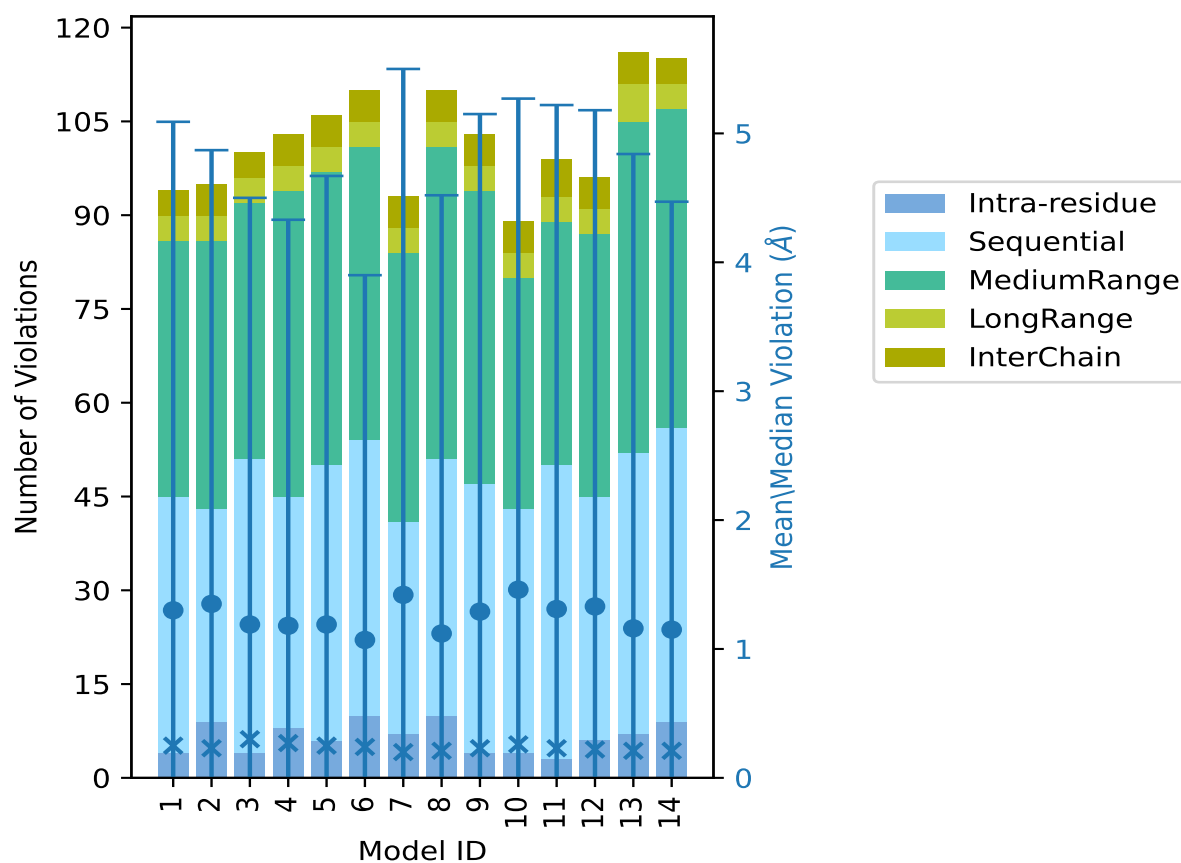
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	47	39	4	6	99	1.31	27.53	3.91	0.23
12	6	39	42	4	5	96	1.33	26.04	3.85	0.22
13	7	45	53	6	5	116	1.16	26.91	3.68	0.21
14	9	47	51	4	4	115	1.15	24.73	3.32	0.21

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

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

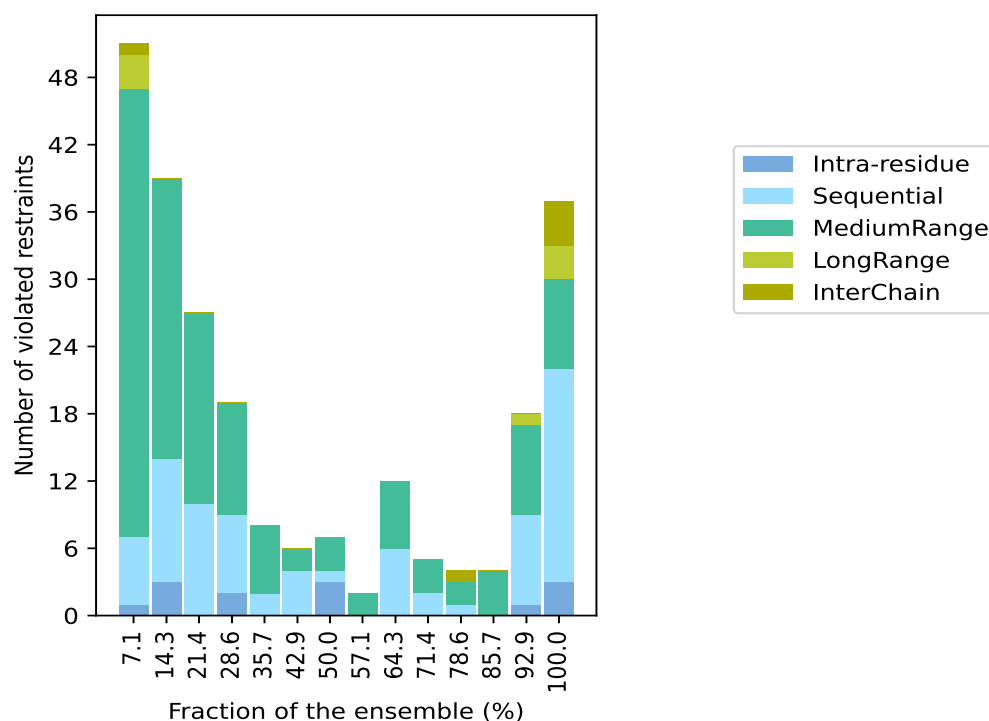
for a given fraction of the ensemble. In total, 430(IR:70, SQ:211, MR:131, LR:18, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	6	40	3	1	51	1	7.1
3	11	25	0	0	39	2	14.3
0	10	17	0	0	27	3	21.4
2	7	10	0	0	19	4	28.6
0	2	6	0	0	8	5	35.7
0	4	2	0	0	6	6	42.9
3	1	3	0	0	7	7	50.0
0	0	2	0	0	2	8	57.1
0	6	6	0	0	12	9	64.3
0	2	3	0	0	5	10	71.4
0	1	2	0	1	4	11	78.6
0	0	4	0	0	4	12	85.7
1	8	8	1	0	18	13	92.9
3	19	8	3	4	37	14	100.0

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

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

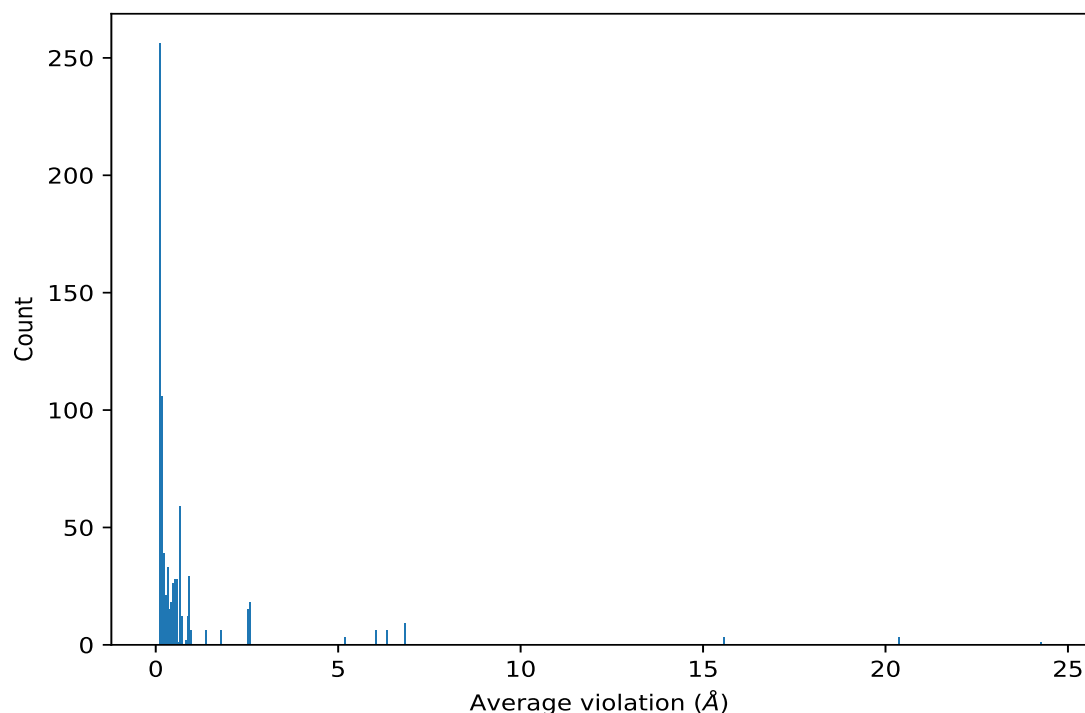
9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	14	24.29	2.67	24.7
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	20.36	1.69	20.49
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	20.36	1.69	20.49
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	20.36	1.69	20.49
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	15.55	1.23	15.22
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	15.55	1.23	15.22
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	15.55	1.23	15.22
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	6.83	0.47	6.74

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	6.83	0.47	6.74
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	6.34	0.65	6.31
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	6.34	0.65	6.31
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	6.34	0.65	6.31
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	6.34	0.65	6.31
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	6.34	0.65	6.31
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	6.34	0.65	6.31
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	6.03	0.56	6.07
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	6.03	0.56	6.07
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	6.03	0.56	6.07
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	6.03	0.56	6.07
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	6.03	0.56	6.07
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	6.03	0.56	6.07
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	5.18	0.91	5.24
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	5.18	0.91	5.24
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	5.18	0.91	5.24
(2,18)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,18)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,18)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	14	2.54	1.27	2.18
(2,18)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	14	2.54	1.27	2.18
(2,18)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,19)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,19)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,19)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	14	2.54	1.27	2.18
(2,19)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	14	2.54	1.27	2.18
(2,19)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,20)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,20)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,20)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	14	2.54	1.27	2.18
(2,20)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	14	2.54	1.27	2.18
(2,20)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	1.78	0.54	1.73
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	1.78	0.54	1.73
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	1.78	0.54	1.73
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	1.78	0.54	1.73
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	1.78	0.54	1.73

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	1.78	0.54	1.73
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	14	0.81	0.16	0.88
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	14	0.81	0.16	0.88
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	14	0.56	0.36	0.45
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	14	0.51	0.09	0.54
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	14	0.51	0.09	0.54
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	14	0.51	0.09	0.54
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	14	0.47	0.03	0.46
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	14	0.47	0.03	0.46
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	14	0.34	0.01	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	14	0.34	0.01	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	14	0.34	0.01	0.34
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	0.32	0.1	0.32
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	0.32	0.1	0.32
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	0.32	0.1	0.32
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	0.32	0.1	0.32
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	0.32	0.1	0.32
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	0.32	0.1	0.32
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	0.32	0.1	0.32
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	0.32	0.1	0.32
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	0.32	0.1	0.32
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	0.32	0.1	0.32
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	14	0.32	0.21	0.24
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	14	0.32	0.21	0.24
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	14	0.32	0.21	0.24
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.23	0.03	0.23
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.23	0.03	0.23
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.23	0.03	0.23
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	14	0.22	0.05	0.21
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.21	0.01	0.21
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.21	0.01	0.21
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.21	0.01	0.21
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	14	0.19	0.06	0.19
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	14	0.19	0.06	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.19	0.03	0.18
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.19	0.03	0.18
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.19	0.03	0.18
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	14	0.19	0.02	0.19
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.18	0.04	0.2
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.18	0.04	0.2
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.18	0.04	0.2
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	14	0.13	0.01	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	14	0.13	0.01	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	14	0.13	0.01	0.13
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	13	2.57	1.05	2.61
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	1.4	0.54	1.66
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	1.4	0.54	1.66
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	1.4	0.54	1.66
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	1.4	0.54	1.66
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	1.4	0.54	1.66
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	1.4	0.54	1.66
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	0.9	0.33	0.98

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	0.9	0.33	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	0.9	0.33	0.98
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.69	0.16	0.65
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.69	0.16	0.65
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.69	0.16	0.65
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.69	0.16	0.65
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.69	0.16	0.65
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.69	0.16	0.65
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	13	0.61	0.19	0.58
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	13	0.58	0.25	0.47
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	13	0.58	0.25	0.47
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	13	0.58	0.25	0.47
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	13	0.58	0.25	0.47
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	13	0.58	0.25	0.47
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	13	0.58	0.25	0.47
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.56	0.08	0.58
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	13	0.56	0.08	0.57
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	13	0.56	0.08	0.57
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	13	0.56	0.08	0.57
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	13	0.56	0.08	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	13	0.56	0.08	0.57
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	13	0.56	0.08	0.57
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	13	0.51	0.15	0.49
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	0.5	0.54	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	0.5	0.54	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	0.5	0.54	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	0.5	0.54	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	0.5	0.54	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	0.5	0.54	0.22
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.46	0.08	0.48
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	13	0.42	0.11	0.43
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	13	0.18	0.05	0.17
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	13	0.18	0.05	0.17
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	13	0.18	0.05	0.17
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	13	0.18	0.05	0.17
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	12	0.7	0.25	0.74
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.68	0.25	0.7
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.68	0.25	0.7
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.68	0.25	0.7
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.68	0.25	0.7
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.68	0.25	0.7
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.68	0.25	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.68	0.25	0.7
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.68	0.25	0.7
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	11	0.69	0.33	0.68
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	11	0.69	0.33	0.68
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	11	0.69	0.33	0.68
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.18	0.05	0.19
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.18	0.05	0.19
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.18	0.05	0.19
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.18	0.05	0.19
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.18	0.05	0.19
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.18	0.05	0.19
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	11	0.14	0.03	0.13
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	11	0.14	0.03	0.13
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	11	0.14	0.03	0.13
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	11	0.14	0.03	0.13
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	11	0.14	0.03	0.13
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	11	0.14	0.03	0.13
(3,638)	1:701:A:VAL:HG11	1:698:A:VAL:HA	10	0.87	0.45	0.7
(3,638)	1:701:A:VAL:HG12	1:698:A:VAL:HA	10	0.87	0.45	0.7
(3,638)	1:701:A:VAL:HG13	1:698:A:VAL:HA	10	0.87	0.45	0.7
(3,638)	1:701:A:VAL:HG21	1:698:A:VAL:HA	10	0.87	0.45	0.7
(3,638)	1:701:A:VAL:HG22	1:698:A:VAL:HA	10	0.87	0.45	0.7
(3,638)	1:701:A:VAL:HG23	1:698:A:VAL:HA	10	0.87	0.45	0.7
(3,597)	1:692:A:LEU:HD11	1:689:A:VAL:HA	10	0.44	0.15	0.52
(3,597)	1:692:A:LEU:HD12	1:689:A:VAL:HA	10	0.44	0.15	0.52
(3,597)	1:692:A:LEU:HD13	1:689:A:VAL:HA	10	0.44	0.15	0.52
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	10	0.19	0.06	0.19
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	10	0.16	0.03	0.16
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	10	0.15	0.03	0.14
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	10	0.15	0.03	0.14
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	10	0.15	0.03	0.14
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	10	0.15	0.03	0.14
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	10	0.15	0.03	0.14
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	10	0.15	0.03	0.14
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	9	0.65	0.3	0.83
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	9	0.65	0.3	0.83

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	9	0.65	0.3	0.83
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	9	0.65	0.3	0.83
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	9	0.65	0.3	0.83
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	9	0.65	0.3	0.83
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	9	0.65	0.3	0.83
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	9	0.55	0.24	0.52
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	9	0.55	0.24	0.52
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	9	0.55	0.24	0.52
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	9	0.55	0.24	0.52
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	9	0.55	0.24	0.52
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	9	0.55	0.24	0.52
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	9	0.51	0.16	0.55
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	9	0.51	0.16	0.55
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	9	0.51	0.16	0.55
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	9	0.51	0.16	0.55
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	9	0.51	0.16	0.55
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	9	0.51	0.16	0.55
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	9	0.5	0.03	0.51
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	9	0.5	0.03	0.51
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	9	0.5	0.03	0.51
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	9	0.5	0.03	0.51
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	9	0.5	0.03	0.51
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	9	0.5	0.03	0.51
(3,543)	1:704:A:LEU:H	1:701:A:VAL:HA	9	0.19	0.05	0.18
(3,180)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,180)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,180)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,393)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,393)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,393)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,606)	1:693:A:ILE:HG21	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,606)	1:693:A:ILE:HG22	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,606)	1:693:A:ILE:HG23	1:694:A:GLY:H	9	0.17	0.03	0.18
(3,132)	1:705:A:VAL:HG11	1:702:A:LEU:HA	9	0.14	0.03	0.13
(3,132)	1:705:A:VAL:HG12	1:702:A:LEU:HA	9	0.14	0.03	0.13
(3,132)	1:705:A:VAL:HG13	1:702:A:LEU:HA	9	0.14	0.03	0.13
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	9	0.14	0.03	0.13
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB2	9	0.13	0.03	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB2	9	0.13	0.03	0.12
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB2	9	0.13	0.03	0.12
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB2	9	0.13	0.03	0.12
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB2	9	0.13	0.03	0.12
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB2	9	0.13	0.03	0.12
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB3	9	0.13	0.03	0.12
(3,174)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	8	0.67	0.14	0.68
(3,174)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	8	0.67	0.14	0.68
(3,174)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	8	0.67	0.14	0.68
(3,174)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	8	0.67	0.14	0.68
(3,174)	1:692:A:LEU:HD13	1:696:A:ARG:HH12	8	0.67	0.14	0.68
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	8	0.51	0.08	0.52
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	8	0.51	0.08	0.52
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	8	0.51	0.08	0.52
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	8	0.51	0.08	0.52
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	8	0.51	0.08	0.52
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	8	0.51	0.08	0.52
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	7	0.23	0.02	0.23
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	7	0.23	0.02	0.23
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	7	0.23	0.02	0.23
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	7	0.23	0.02	0.23
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	7	0.23	0.02	0.23
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	7	0.23	0.02	0.23
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	7	0.22	0.05	0.22
(3,499)	1:678:A:TRP:HE1	1:682:A:ILE:H	7	0.22	0.05	0.22
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	7	0.19	0.04	0.17
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	7	0.19	0.04	0.17
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	7	0.19	0.04	0.17
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	7	0.19	0.04	0.17
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	7	0.19	0.04	0.17
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	7	0.19	0.04	0.17
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.18	0.07	0.16
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.18	0.07	0.16
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.18	0.07	0.16
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.18	0.07	0.16
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.18	0.07	0.16
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.18	0.07	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,349)	1:705:A:VAL:HG21	1:702:A:LEU:HG	6	0.44	0.32	0.29
(3,349)	1:705:A:VAL:HG22	1:702:A:LEU:HG	6	0.44	0.32	0.29
(3,349)	1:705:A:VAL:HG23	1:702:A:LEU:HG	6	0.44	0.32	0.29
(3,551)	1:704:A:LEU:HD11	1:707:A:ARG:HE	6	0.43	0.12	0.48
(3,551)	1:704:A:LEU:HD12	1:707:A:ARG:HE	6	0.43	0.12	0.48
(3,551)	1:704:A:LEU:HD13	1:707:A:ARG:HE	6	0.43	0.12	0.48
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	6	0.26	0.03	0.24
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	6	0.26	0.03	0.24
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	6	0.26	0.03	0.24
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	6	0.26	0.03	0.24
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	6	0.26	0.03	0.24
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	6	0.26	0.03	0.24
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	6	0.26	0.03	0.24
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.16	0.03	0.16
(3,245)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.16	0.03	0.16
(3,458)	1:667:A:ALA:H	1:666:A:TRP:HD1	6	0.16	0.03	0.16
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	5	0.66	0.19	0.73
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	5	0.66	0.19	0.73
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	5	0.66	0.19	0.73
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	5	0.66	0.19	0.73
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	5	0.66	0.19	0.73
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	5	0.66	0.19	0.73
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	5	0.66	0.19	0.73
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	5	0.66	0.19	0.73
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	5	0.66	0.19	0.73
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	5	0.42	0.31	0.25
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	5	0.42	0.31	0.25
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	5	0.42	0.31	0.25
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	5	0.42	0.31	0.25
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	5	0.42	0.31	0.25
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	5	0.42	0.31	0.25
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	5	0.38	0.13	0.39
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	5	0.38	0.13	0.39
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	5	0.38	0.13	0.39
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	5	0.38	0.13	0.39
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	5	0.38	0.13	0.39
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	5	0.38	0.13	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	5	0.38	0.13	0.39
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	5	0.38	0.13	0.39
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	5	0.38	0.13	0.39
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	5	0.15	0.02	0.15
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	5	0.15	0.02	0.15
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	5	0.15	0.02	0.15
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	5	0.15	0.02	0.15
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	5	0.15	0.02	0.15
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	5	0.15	0.02	0.15
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	5	0.14	0.02	0.14
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	5	0.14	0.02	0.14
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	5	0.13	0.03	0.12
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	5	0.13	0.03	0.12
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	5	0.13	0.03	0.12
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	5	0.13	0.01	0.13
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	5	0.13	0.01	0.13
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	5	0.13	0.01	0.13
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	5	0.13	0.01	0.13
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	5	0.13	0.01	0.13
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	5	0.13	0.01	0.13
(3,561)	1:705:A:VAL:HG21	1:701:A:VAL:HA	4	0.6	0.06	0.6
(3,561)	1:705:A:VAL:HG22	1:701:A:VAL:HA	4	0.6	0.06	0.6
(3,561)	1:705:A:VAL:HG23	1:701:A:VAL:HA	4	0.6	0.06	0.6
(3,289)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	4	0.4	0.24	0.3
(3,289)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	4	0.4	0.24	0.3
(3,193)	1:697:A:ILE:HG21	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,193)	1:697:A:ILE:HG22	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,193)	1:697:A:ILE:HG23	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,406)	1:697:A:ILE:HG21	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,406)	1:697:A:ILE:HG22	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,406)	1:697:A:ILE:HG23	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,619)	1:697:A:ILE:HG21	1:698:A:VAL:HA	4	0.34	0.01	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,619)	1:697:A:ILE:HG22	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,619)	1:697:A:ILE:HG23	1:698:A:VAL:HA	4	0.34	0.01	0.34
(3,15)	1:665:A:LYS:H	1:662:A:GLU:HA	4	0.22	0.09	0.2
(3,228)	1:665:A:LYS:H	1:662:A:GLU:HA	4	0.22	0.09	0.2
(3,441)	1:665:A:LYS:H	1:662:A:GLU:HA	4	0.22	0.09	0.2
(3,173)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,173)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,173)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,173)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,173)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,173)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,386)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,386)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,386)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,386)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,386)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,386)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,599)	1:692:A:LEU:HD11	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,599)	1:692:A:LEU:HD11	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,599)	1:692:A:LEU:HD12	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,599)	1:692:A:LEU:HD12	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,599)	1:692:A:LEU:HD13	1:691:A:SER:HB2	4	0.18	0.04	0.18
(3,599)	1:692:A:LEU:HD13	1:691:A:SER:HB3	4	0.18	0.04	0.18
(3,46)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.16	0.01	0.16
(3,259)	1:670:A:TRP:H	1:667:A:ALA:HA	4	0.16	0.01	0.16
(3,404)	1:696:A:ARG:H	1:696:A:ARG:HE	4	0.16	0.03	0.15
(3,617)	1:696:A:ARG:H	1:696:A:ARG:HE	4	0.16	0.03	0.15
(3,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,301)	1:684:A:ILE:HD11	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,301)	1:684:A:ILE:HD12	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,301)	1:684:A:ILE:HD13	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,514)	1:684:A:ILE:HD11	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,514)	1:684:A:ILE:HD12	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,514)	1:684:A:ILE:HD13	1:681:A:TYR:HA	4	0.14	0.03	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	4	0.13	0.02	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	4	0.13	0.02	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	4	0.13	0.02	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	4	0.13	0.02	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	4	0.13	0.02	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	4	0.13	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,345)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,345)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,345)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,558)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,558)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,558)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	0.96	0.09	0.99
(3,502)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	3	0.95	0.06	0.95
(3,502)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	3	0.95	0.06	0.95
(3,389)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,389)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,389)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,389)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,389)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,389)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,602)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,602)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,602)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,602)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,602)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	3	0.71	0.03	0.7
(3,602)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	3	0.71	0.03	0.7
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD11	3	0.38	0.14	0.45
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD12	3	0.38	0.14	0.45
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD13	3	0.38	0.14	0.45
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD21	3	0.38	0.14	0.45
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD22	3	0.38	0.14	0.45
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD23	3	0.38	0.14	0.45
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	3	0.16	0.04	0.14
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	3	0.16	0.04	0.14
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	3	0.16	0.04	0.14
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	3	0.16	0.04	0.14
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	3	0.16	0.04	0.14
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	3	0.16	0.04	0.14
(3,562)	1:705:A:VAL:HG21	1:702:A:LEU:HG	3	0.16	0.05	0.13
(3,562)	1:705:A:VAL:HG22	1:702:A:LEU:HG	3	0.16	0.05	0.13
(3,562)	1:705:A:VAL:HG23	1:702:A:LEU:HG	3	0.16	0.05	0.13
(3,53)	1:671:A:ASN:H	1:672:A:TRP:HE1	3	0.15	0.04	0.13
(3,57)	1:672:A:TRP:HE1	1:671:A:ASN:H	3	0.15	0.04	0.13
(3,266)	1:671:A:ASN:H	1:672:A:TRP:HE1	3	0.15	0.04	0.13
(3,270)	1:672:A:TRP:HE1	1:671:A:ASN:H	3	0.15	0.04	0.13
(3,177)	1:693:A:ILE:HD11	1:697:A:ILE:H	3	0.15	0.02	0.14
(3,177)	1:693:A:ILE:HD12	1:697:A:ILE:H	3	0.15	0.02	0.14
(3,177)	1:693:A:ILE:HD13	1:697:A:ILE:H	3	0.15	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	3	0.14	0.05	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	3	0.14	0.05	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	3	0.14	0.05	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	3	0.14	0.05	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	3	0.14	0.05	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	3	0.14	0.05	0.1
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	3	0.13	0.01	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	3	0.13	0.01	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	3	0.13	0.01	0.14
(3,127)	1:705:A:VAL:H	1:702:A:LEU:HA	3	0.13	0.01	0.12
(3,340)	1:705:A:VAL:H	1:702:A:LEU:HA	3	0.13	0.01	0.12
(3,196)	1:698:A:VAL:HG11	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,196)	1:698:A:VAL:HG12	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,196)	1:698:A:VAL:HG13	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,409)	1:698:A:VAL:HG11	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,409)	1:698:A:VAL:HG12	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,409)	1:698:A:VAL:HG13	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,622)	1:698:A:VAL:HG11	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,622)	1:698:A:VAL:HG12	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,622)	1:698:A:VAL:HG13	1:695:A:LEU:HG	3	0.12	0.0	0.12
(3,79)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11	0.0	0.11
(3,186)	1:695:A:LEU:HD21	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,186)	1:695:A:LEU:HD22	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,186)	1:695:A:LEU:HD23	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,292)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11	0.0	0.11
(3,399)	1:695:A:LEU:HD21	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,399)	1:695:A:LEU:HD22	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,399)	1:695:A:LEU:HD23	1:698:A:VAL:HB	3	0.11	0.01	0.1
(3,505)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11	0.0	0.11
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	2	0.88	0.18	0.88
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	2	0.88	0.18	0.88
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	2	0.88	0.18	0.88
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	2	0.88	0.18	0.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	2	0.88	0.18	0.88
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	2	0.88	0.18	0.88
(3,375)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,375)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,375)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,375)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,375)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,375)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,375)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,375)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,375)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,588)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,588)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,588)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,588)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,588)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,588)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,588)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	2	0.48	0.24	0.48
(3,588)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	2	0.48	0.24	0.48
(3,588)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	2	0.48	0.24	0.48
(3,78)	1:681:A:TYR:H	1:680:A:TRP:H	2	0.29	0.01	0.29
(3,291)	1:681:A:TYR:H	1:680:A:TRP:H	2	0.29	0.01	0.29
(3,504)	1:681:A:TYR:H	1:680:A:TRP:H	2	0.29	0.01	0.29
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD11	2	0.29	0.06	0.29
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD12	2	0.29	0.06	0.29
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD13	2	0.29	0.06	0.29
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD21	2	0.29	0.06	0.29
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD22	2	0.29	0.06	0.29
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD23	2	0.29	0.06	0.29
(3,150)	1:707:A:ARG:H	1:707:A:ARG:HG2	2	0.21	0.01	0.21
(3,150)	1:707:A:ARG:H	1:707:A:ARG:HG3	2	0.21	0.01	0.21
(3,363)	1:707:A:ARG:H	1:707:A:ARG:HG2	2	0.21	0.01	0.21
(3,363)	1:707:A:ARG:H	1:707:A:ARG:HG3	2	0.21	0.01	0.21
(3,576)	1:707:A:ARG:H	1:707:A:ARG:HG2	2	0.21	0.01	0.21
(3,576)	1:707:A:ARG:H	1:707:A:ARG:HG3	2	0.21	0.01	0.21
(3,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,80)	1:682:A:ILE:HG21	1:679:A:LEU:H	2	0.2	0.04	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,80)	1:682:A:ILE:HG22	1:679:A:LEU:H	2	0.2	0.04	0.2
(3,80)	1:682:A:ILE:HG23	1:679:A:LEU:H	2	0.2	0.04	0.2
(3,288)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,288)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,288)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,288)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,288)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,288)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	2	0.2	0.03	0.2
(3,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	2	0.18	0.01	0.18
(3,40)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.18	0.08	0.18
(3,233)	1:665:A:LYS:H	1:666:A:TRP:HD1	2	0.18	0.01	0.18
(3,253)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.18	0.08	0.18
(3,446)	1:665:A:LYS:H	1:666:A:TRP:HD1	2	0.18	0.01	0.18
(3,466)	1:669:A:LEU:H	1:666:A:TRP:HA	2	0.18	0.08	0.18
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD11	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD12	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD13	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD21	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD22	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD23	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD11	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD12	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD13	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD21	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD22	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD23	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD11	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD12	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD13	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD21	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD22	2	0.16	0.01	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD23	2	0.16	0.01	0.16
(3,165)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,165)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,165)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,378)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,378)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,378)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,591)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,591)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,591)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.15	0.01	0.15
(3,135)	1:705:A:VAL:HG21	1:701:A:VAL:HA	2	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,135)	1:705:A:VAL:HG22	1:701:A:VAL:HA	2	0.14	0.03	0.14
(3,135)	1:705:A:VAL:HG23	1:701:A:VAL:HA	2	0.14	0.03	0.14
(3,348)	1:705:A:VAL:HG21	1:701:A:VAL:HA	2	0.14	0.03	0.14
(3,348)	1:705:A:VAL:HG22	1:701:A:VAL:HA	2	0.14	0.03	0.14
(3,348)	1:705:A:VAL:HG23	1:701:A:VAL:HA	2	0.14	0.03	0.14
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,192)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	2	0.14	0.02	0.14
(3,192)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	2	0.14	0.02	0.14
(3,192)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	2	0.14	0.02	0.14
(3,192)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	2	0.14	0.02	0.14
(3,192)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	2	0.14	0.02	0.14
(3,192)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	2	0.14	0.02	0.14
(3,515)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,515)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,515)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,515)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,515)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	2	0.14	0.01	0.14
(3,515)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	2	0.14	0.01	0.14
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,176)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(3,176)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(3,176)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(3,176)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(3,176)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	2	0.12	0.02	0.12
(3,176)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	2	0.12	0.02	0.12
(3,295)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	2	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,295)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,295)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,295)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,295)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,295)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,508)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,508)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,508)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,508)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,508)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,508)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,518)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,518)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,518)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,518)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,518)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	2	0.12	0.02	0.12
(3,518)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	2	0.12	0.02	0.12
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,222)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,222)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	2	0.12	0.02	0.12
(3,222)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,222)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,222)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	2	0.12	0.02	0.12
(3,222)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,222)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	2	0.12	0.02	0.12
(3,222)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	2	0.12	0.02	0.12
(3,222)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	2	0.12	0.02	0.12
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	2	0.11	0.0	0.11
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	2	0.11	0.0	0.11
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	2	0.11	0.0	0.11
(3,263)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	2	0.11	0.0	0.11
(3,263)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	2	0.11	0.0	0.11
(3,263)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	2	0.11	0.0	0.11
(3,476)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	2	0.11	0.0	0.11

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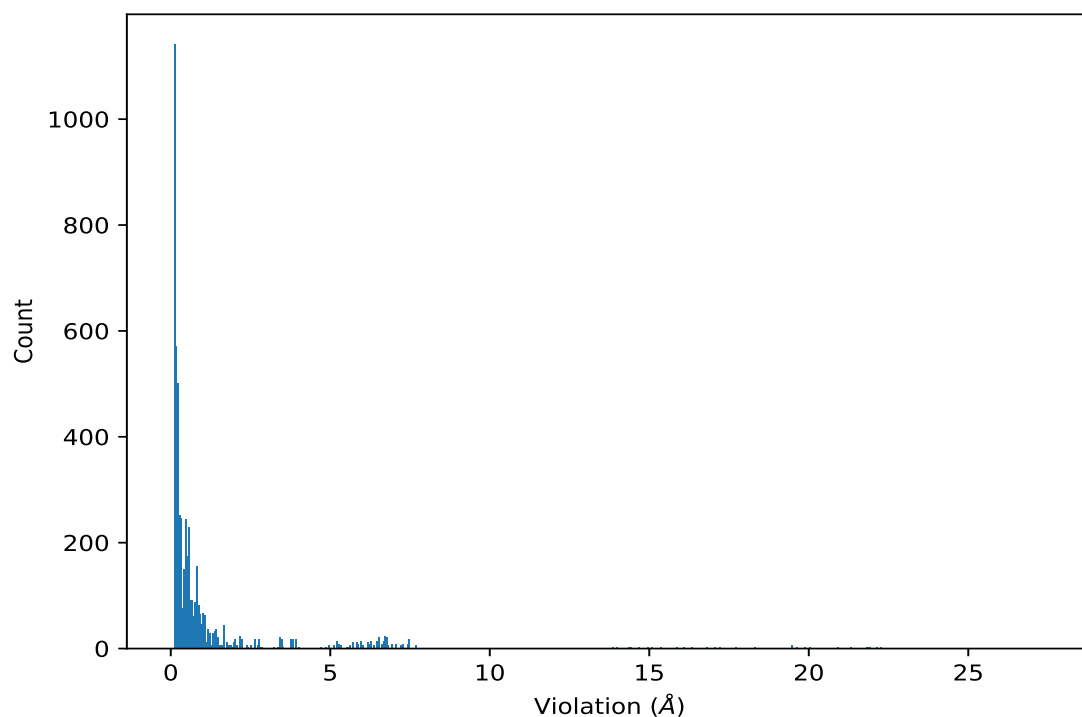
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,476)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	2	0.11	0.0	0.11
(3,476)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	11	27.53
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	9	27.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	13	26.91
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	7	26.6
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	12	26.04
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	8	25.21
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	14	24.73
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	10	24.66
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	5	24.63
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	1	24.54
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	7	22.26
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	7	22.26
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	7	22.26
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	13	22.12
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	13	22.12
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	13	22.12
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	3	22.03
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	9	21.95
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	9	21.95
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	9	21.95
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	12	21.86
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	12	21.86
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	12	21.86
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	1	21.81
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	1	21.81
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	1	21.81
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	2	21.48
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	11	21.32
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	11	21.32
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	11	21.32
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	5	20.95
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	5	20.95
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	5	20.95
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	4	20.42
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	8	20.03
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	8	20.03
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	8	20.03
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	10	19.88
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	10	19.88
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	10	19.88
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	2	19.6
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	2	19.6
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	2	19.6
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	3	19.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	3	19.46
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	3	19.46
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	19.46
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	19.46
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	19.46
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	4	18.34
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	4	18.34
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	4	18.34
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	6	18.2
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	13	17.71
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	13	17.71
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	13	17.71
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	7	17.21
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	7	17.21
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	7	17.21
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	9	17.09
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	9	17.09
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	9	17.09
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	11	16.8
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	11	16.8
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	11	16.8
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	2	16.3
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	2	16.3
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	2	16.3
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	6	16.07
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	6	16.07
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	6	16.07
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	1	15.87
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	1	15.87
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	1	15.87
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	12	15.38
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	12	15.38
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	12	15.38
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	15.06
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	15.06
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	15.06
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	10	14.98
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	10	14.98
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	10	14.98
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	5	14.65
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	5	14.65
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	5	14.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	6	14.44
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	6	14.44
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	6	14.44
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	4	14.37
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	4	14.37
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	4	14.37
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	3	13.98
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	3	13.98
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	3	13.98
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	8	13.88
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	8	13.88
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	8	13.88
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	7.66
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	7.66
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	7.66
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	7.66
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	6	7.66
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	6	7.66
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	7.47
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	7.47
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	7.47
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	7.47
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	7.47
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	7.47
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	1	7.47
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	1	7.47
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	1	7.47
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	7.46
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	7.46
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	7.46
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	7.46
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	7.46
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	7.46
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	7	7.46
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	7	7.46
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	7	7.46
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	7.43
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	7.43
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	7.43
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	7.43
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	7.43
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	7.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	3	7.43
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	3	7.43
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	3	7.43
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	7.28
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	7.28
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	7.28
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	7.28
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	7.28
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	7.28
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	13	7.28
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	13	7.28
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	13	7.28
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	7.2
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	7.2
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	7.2
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	7.2
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	2	7.2
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	2	7.2
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	7.08
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	7.08
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	7.08
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	7.08
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	7.08
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	7.08
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	2	7.08
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	2	7.08
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	2	7.08
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	6.9
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	6.9
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	6.9
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	6.9
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	6.9
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	6.9
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	12	6.9
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	12	6.9
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	12	6.9
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	6.82
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	6.82
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	6.82
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	6.82
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	7	6.82
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	7	6.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	6	6.79
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	6	6.79
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	6	6.79
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	6	6.79
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	6	6.79
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	6	6.79
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	6.76
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	6.76
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	6.76
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	6.76
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	6.76
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	6.76
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	4	6.76
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	4	6.76
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	4	6.76
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	9	6.76
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	9	6.76
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	9	6.76
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	9	6.76
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	9	6.76
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	9	6.76
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	6.74
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	6.74
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	6.74
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	6.74
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	8	6.74
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	8	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	6.73
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	6.73
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	6.73
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	6.73
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	6.73
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	6.73
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	6.73
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	6.73
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	6.73
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	6.7
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	6.7
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	6.7
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	6.7
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	6.7
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	6.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	5	6.7
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	5	6.7
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	5	6.7
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	6.68
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	6.68
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	13	6.68
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	6.68
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	6.68
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	6.68
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	6.68
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	11	6.68
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	11	6.68
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	4	6.68
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	4	6.68
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	4	6.68
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	4	6.68
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	4	6.68
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	4	6.68
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	6.63
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	6.63
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	6.63
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	6.63
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	6.63
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	6.63
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	6	6.63
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	6	6.63
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	6	6.63
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	6.54
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	6.54
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	6.54
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	6.54
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	4	6.54
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	4	6.54
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	6.53
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	6.53
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	6.53
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	6.53
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	6.53
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	6.53
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	9	6.53
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	9	6.53
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	9	6.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	8	6.52
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	8	6.52
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	8	6.52
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	8	6.52
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	8	6.52
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	8	6.52
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	6.48
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	6.48
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	6.48
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	6.48
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	6.48
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	6.48
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	11	6.48
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	11	6.48
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	11	6.48
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	7	6.48
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	7	6.48
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	7	6.48
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	7	6.48
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	7	6.48
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	7	6.48
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	6.39
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	6.39
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	6.39
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	6.39
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	10	6.39
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	10	6.39
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	3	6.28
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	3	6.28
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	3	6.28
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	3	6.28
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	3	6.28
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	3	6.28
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	6.27
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	6.27
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	6.27
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	6.27
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	6.27
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	6.27
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	10	6.27
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	10	6.27
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	10	6.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	6.23
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	6.23
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	6.23
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	6.23
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	12	6.23
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	12	6.23
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	6.2
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	6.2
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	2	6.2
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	2	6.19
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	2	6.19
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	2	6.19
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	2	6.19
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	2	6.19
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	2	6.19
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	6.16
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	6.16
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	6.16
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	6.16
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	9	6.16
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	9	6.16
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	6.05
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	6.05
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	6.05
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	6.05
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	5	6.05
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	5	6.05
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	5.98
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	5.98
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	5.98
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	5.98
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	1	5.98
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	1	5.98
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	5.96
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	5.96
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	9	5.96
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	12	5.95
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	12	5.95
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	12	5.95
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	12	5.95
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	12	5.95
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	12	5.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	10	5.86
(2,19)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	10	5.86
(2,18)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	10	5.86
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	5.86
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	5.86
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	5.86
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	5.86
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	5.86
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	5.86
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	5.84
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	5.84
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	1	5.84
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	5.83
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	5.83
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	5.83
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	5.83
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	5.83
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	5.83
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	8	5.83
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	8	5.83
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	8	5.83
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	11	5.72
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	11	5.72
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	11	5.72
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	11	5.72
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	11	5.72
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	11	5.72
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	13	5.7
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	13	5.7
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	13	5.7
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	13	5.7
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	13	5.7
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	13	5.7
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	1	5.63
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	1	5.63
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	1	5.63
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	1	5.63
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	1	5.63
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	1	5.63
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	5.56
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	5.56
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	5.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	5.5
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	5.5
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	12	5.5
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	5	5.33
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	5	5.33
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	5	5.33
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	5	5.33
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	5	5.33
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	5	5.33
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	5.29
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	5.29
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	5.29
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	5.29
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	3	5.29
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	3	5.29
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	5.26
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	5.26
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	11	5.26
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	5.23
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	5.23
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	3	5.23
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	5.22
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	5.22
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	5.22
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	5.22
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	13	5.22
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	13	5.22
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	5.2
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	5.2
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	5.2
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	5.2
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	5.2
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	5.2
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	10	5.13
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	10	5.13
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	10	5.13
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	10	5.13
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	10	5.13
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	10	5.13
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	4.98
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	4.98
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	7	4.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	4.97
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	4.97
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	10	4.97
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	4.89
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	4.89
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	4	4.89
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	4.7
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	4.7
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	5	4.7
(2,20)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	7	4.04
(2,19)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	7	4.04
(2,18)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	7	4.04
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	4	3.93
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	3.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	12	3.83
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	9	3.77
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	9	3.77
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	3.55
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	3.55
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	6	3.55
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	5	3.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	5	3.47
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	5	3.47
(2,20)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	2	3.44
(2,19)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	2	3.44
(2,18)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	2	3.44
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	11	3.41
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	11	3.41
(2,20)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	3.39
(2,19)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	3.39
(2,18)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	3.39
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	3.2
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	3.2
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	8	3.2
(2,20)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	6	2.87
(2,19)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	6	2.87
(2,18)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	6	2.87
(2,20)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	13	2.82
(2,19)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	13	2.82
(2,18)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	13	2.82
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	2.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	8	2.8
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	8	2.8
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	2.71
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	2.71
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	2.71
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	2.71
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	4	2.71
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	4	2.71
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	14	2.61
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	14	2.61
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	2.5
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	2.5
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	2.5
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	2.5
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	11	2.5
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	11	2.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	8	2.43
(2,19)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	8	2.43
(2,18)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	8	2.43
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	2.38
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	2.38
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	2.38
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	2.38
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	7	2.38
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	7	2.38
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	6	2.2
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	6	2.2
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	2.18
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	2.18
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	2.18
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	2.18
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	10	2.18
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	10	2.18
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	2.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	3	2.17
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	3	2.17
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	2.06
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	2.06
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	2.06
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	2.06
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	2	2.06
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	2	2.06
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	10	2.0
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	10	2.0
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	1.99
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	1.99
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	1.99
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	1.99
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	8	1.99
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	8	1.99
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	1.98
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	1.98
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	1.98
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	14	1.98
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	14	1.98
(2,20)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	12	1.94
(2,19)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	12	1.94
(2,18)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	12	1.94
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	1.88
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	1.88
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	1.88
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	1.88
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	2	1.88
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	2	1.88
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	1.8
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	1.8
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	1.8
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	1.8
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	12	1.8
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	12	1.8
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	1.79
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	1.79
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	1.79
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	1.79
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	10	1.79
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	10	1.79
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	1.78
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	1.78
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	1.78
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	1.78
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	5	1.78
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	5	1.78
(2,20)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	5	1.69
(2,19)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	5	1.69
(2,18)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	5	1.69
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	7	1.69
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	7	1.69
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	1.68
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	1.68
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	1.68
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	1.68
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	8	1.68
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	8	1.68
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	1.68
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	1.68
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	1.68
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	1.68
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	9	1.68
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	9	1.68
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	1.67
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	1.67
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	1.67
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	1.67
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	9	1.67
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	9	1.67
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	1.66
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	1.66
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	1.66
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	1.66
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	5	1.66
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	5	1.66
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	1.62
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	1.62
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	1.62
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	1.62
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	14	1.62
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	14	1.62
(2,20)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	3	1.59
(2,20)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	11	1.59
(2,19)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	3	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	11	1.59
(2,18)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	3	1.59
(2,18)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	11	1.59
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	2	1.51
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	2	1.51
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	2	1.51
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	2	1.51
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	2	1.51
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	2	1.51
(2,20)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	9	1.49
(2,19)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	9	1.49
(2,18)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	9	1.49
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	1.49
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	1.49
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	1.49
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	1.49
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	12	1.49
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	12	1.49
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	1.48
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	1.48
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	1.48
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	1.48
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	6	1.48
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	6	1.48
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	10	1.48
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	10	1.48
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	10	1.48
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	10	1.48
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	10	1.48
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	10	1.48
(3,638)	1:701:A:VAL:HG11	1:698:A:VAL:HA	2	1.45
(3,638)	1:701:A:VAL:HG12	1:698:A:VAL:HA	2	1.45
(3,638)	1:701:A:VAL:HG13	1:698:A:VAL:HA	2	1.45
(3,638)	1:701:A:VAL:HG21	1:698:A:VAL:HA	2	1.45
(3,638)	1:701:A:VAL:HG22	1:698:A:VAL:HA	2	1.45
(3,638)	1:701:A:VAL:HG23	1:698:A:VAL:HA	2	1.45
(3,638)	1:701:A:VAL:HG11	1:698:A:VAL:HA	4	1.45
(3,638)	1:701:A:VAL:HG12	1:698:A:VAL:HA	4	1.45
(3,638)	1:701:A:VAL:HG13	1:698:A:VAL:HA	4	1.45
(3,638)	1:701:A:VAL:HG21	1:698:A:VAL:HA	4	1.45
(3,638)	1:701:A:VAL:HG22	1:698:A:VAL:HA	4	1.45
(3,638)	1:701:A:VAL:HG23	1:698:A:VAL:HA	4	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,638)	1:701:A:VAL:HG11	1:698:A:VAL:HA	14	1.45
(3,638)	1:701:A:VAL:HG12	1:698:A:VAL:HA	14	1.45
(3,638)	1:701:A:VAL:HG13	1:698:A:VAL:HA	14	1.45
(3,638)	1:701:A:VAL:HG21	1:698:A:VAL:HA	14	1.45
(3,638)	1:701:A:VAL:HG22	1:698:A:VAL:HA	14	1.45
(3,638)	1:701:A:VAL:HG23	1:698:A:VAL:HA	14	1.45
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	14	1.44
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	14	1.44
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	14	1.44
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	14	1.44
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	14	1.44
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	14	1.44
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	1.42
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	1.42
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	1.42
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	1.42
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	13	1.42
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	13	1.42
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	1.41
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	1.41
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	1.41
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	1.41
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	1	1.41
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	1	1.41
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	1.38
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	1.38
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	1.38
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	1.38
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	1	1.38
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	1	1.38
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	1.37
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	1.37
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	1.37
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	1.37
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	1.37
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	1.37
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	1.37
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	1.37
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	1.37
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	1.37
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	1.37
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	1.37
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	1.37
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	1.37
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	1.37
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	1.37
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	1.37
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	6	1.37
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	6	1.37
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	6	1.37
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	6	1.37
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	6	1.37
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	6	1.37
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	6	1.37
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	6	1.37
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	6	1.37
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	11	1.33
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	11	1.33
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	11	1.33
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	1.32
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	1.32
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	1.32
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	1.32
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	1.32
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	1.32
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	11	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	11	1.32
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	11	1.32
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	11	1.32
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	4	1.28
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	1.26
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	1.26
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	1.26
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	1.26
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	11	1.26
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	11	1.26
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	1.22
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	1.22
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	1.22
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	1.22
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	1.22
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	1.22
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	1.22
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	1.22
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	1.22
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	1.22
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	1.22
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	1.22
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	1.22
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	1.22
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	1.22
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	1.22
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	1.22
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	1.22
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	5	1.22
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	5	1.22
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	5	1.22
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	5	1.22
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	5	1.22
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	5	1.22
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	5	1.22
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	5	1.22
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	5	1.22
(2,20)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	4	1.21
(2,19)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	4	1.21
(2,18)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	4	1.21
(2,20)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	1	1.2
(2,19)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	1	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,18)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	1	1.2
(3,638)	1:701:A:VAL:HG11	1:698:A:VAL:HA	13	1.19
(3,638)	1:701:A:VAL:HG12	1:698:A:VAL:HA	13	1.19
(3,638)	1:701:A:VAL:HG13	1:698:A:VAL:HA	13	1.19
(3,638)	1:701:A:VAL:HG21	1:698:A:VAL:HA	13	1.19
(3,638)	1:701:A:VAL:HG22	1:698:A:VAL:HA	13	1.19
(3,638)	1:701:A:VAL:HG23	1:698:A:VAL:HA	13	1.19
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	3	1.18
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	1.18
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	1.18
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	1.18
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	1.18
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	1.18
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	1.18
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	1.18
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	1.18
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	1.18
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	1.18
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	1.18
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	1.18
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	1.18
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	1.18
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	1.18
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	1.18
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	1.18
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	1.18
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	2	1.18
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	2	1.18
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	2	1.18
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	2	1.18
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	2	1.18
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	2	1.18
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	2	1.18
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	2	1.18
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	2	1.18
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	1.13
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	1.13
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	1.13
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	1.13
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	7	1.13
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	7	1.13
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	12	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	12	1.13
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	12	1.13
(3,349)	1:705:A:VAL:HG21	1:702:A:LEU:HG	8	1.12
(3,349)	1:705:A:VAL:HG22	1:702:A:LEU:HG	8	1.12
(3,349)	1:705:A:VAL:HG23	1:702:A:LEU:HG	8	1.12
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	1	1.09
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	13	1.08
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	13	1.08
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	13	1.08
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	13	1.08
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	13	1.08
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	13	1.08
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	13	1.08
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	13	1.08
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	13	1.08
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	13	1.08
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	13	1.08
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	13	1.08
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	13	1.08
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	13	1.08
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	13	1.08
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	13	1.08
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	13	1.08
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	13	1.08
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	2	1.07
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	2	1.07
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	2	1.07
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	2	1.07
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	2	1.07
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	2	1.07
(3,558)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	1.06
(3,558)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	1.06
(3,558)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	1.06
(3,345)	1:705:A:VAL:HG11	1:702:A:LEU:HA	3	1.06
(3,345)	1:705:A:VAL:HG12	1:702:A:LEU:HA	3	1.06
(3,345)	1:705:A:VAL:HG13	1:702:A:LEU:HA	3	1.06
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	11	1.06
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	11	1.06
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	11	1.06
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	11	1.06
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	11	1.06
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	11	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	1.05
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	1.05
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	1.05
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	1.05
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	1.05
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	1.05
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	1.05
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	1.05
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	1.05
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	1.05
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	1.05
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	1.05
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	1.05
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	1.05
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	1.05
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	1.05
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	1.05
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	1.05
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	1	1.05
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	1	1.05
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	1	1.05
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	1	1.05
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	1	1.05
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	1	1.05
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	1	1.05
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	1	1.05
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	1	1.05
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	1.03
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	1.03
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	1.03
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	1.03
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	1.03
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	1.03
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	1.03
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	1.03
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	1.03
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	1.03
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	1.03
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	1.03
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	1.03
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	1.03
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	1.03
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	1.03
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	1.03
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	3	1.03
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	3	1.03
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	3	1.03
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	3	1.03
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	3	1.03
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	3	1.03
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	3	1.03
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	3	1.03
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	3	1.03
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	5	1.02
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	5	1.02
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	5	1.02
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	5	1.02
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	5	1.02
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	5	1.02
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	4	1.02
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	4	1.02
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	4	1.02
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	4	1.02
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	4	1.02
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	4	1.02
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	4	1.02
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	4	1.02
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	4	1.02
(3,502)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	5	1.02
(3,502)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	5	1.02
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	4	1.02
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	4	1.02
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	4	1.02
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	4	1.02
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	4	1.02
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	4	1.02
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	4	1.02
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	4	1.02
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	4	1.02
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	7	1.01
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	7	1.01
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	7	1.01
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	9	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	9	1.01
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	9	1.01
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	7	1.01
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	7	1.01
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	7	1.01
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	9	1.01
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	9	1.01
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	9	1.01
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	3	1.0
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	3	1.0
(3,558)	1:705:A:VAL:HG11	1:702:A:LEU:HA	1	0.99
(3,558)	1:705:A:VAL:HG12	1:702:A:LEU:HA	1	0.99
(3,558)	1:705:A:VAL:HG13	1:702:A:LEU:HA	1	0.99
(3,345)	1:705:A:VAL:HG11	1:702:A:LEU:HA	1	0.99
(3,345)	1:705:A:VAL:HG12	1:702:A:LEU:HA	1	0.99
(3,345)	1:705:A:VAL:HG13	1:702:A:LEU:HA	1	0.99
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	0.99
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	0.99
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	0.99
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	0.99
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	6	0.99
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	6	0.99
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	14	0.98
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	14	0.98
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	14	0.98
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	14	0.98
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	14	0.98
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	14	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	12	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	12	0.98
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	12	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	12	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	12	0.98
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	12	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	12	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	12	0.98
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	12	0.98
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	5	0.97
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	5	0.97
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	1	0.95
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	1	0.95
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	1	0.95
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	1	0.95
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	1	0.95
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	1	0.95
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	4	0.95
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	4	0.95
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	4	0.95
(3,502)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	6	0.95
(3,502)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	6	0.95
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	4	0.95
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	4	0.95
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	4	0.95
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	7	0.94
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	7	0.94
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	1	0.93
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	1	0.93
(3,638)	1:701:A:VAL:HG11	1:698:A:VAL:HA	6	0.92
(3,638)	1:701:A:VAL:HG12	1:698:A:VAL:HA	6	0.92
(3,638)	1:701:A:VAL:HG13	1:698:A:VAL:HA	6	0.92
(3,638)	1:701:A:VAL:HG21	1:698:A:VAL:HA	6	0.92
(3,638)	1:701:A:VAL:HG22	1:698:A:VAL:HA	6	0.92
(3,638)	1:701:A:VAL:HG23	1:698:A:VAL:HA	6	0.92
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	12	0.92
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	13	0.92
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	12	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	13	0.92
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	1	0.91
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	1	0.91
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	1	0.91
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	1	0.91
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	1	0.91
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	1	0.91
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	14	0.91
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	14	0.91
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	14	0.91
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	14	0.91
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	14	0.91
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	14	0.91
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	13	0.91
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	13	0.91
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	13	0.91
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	13	0.91
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	13	0.91
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	13	0.91
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	9	0.9
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	9	0.9
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	9	0.9
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	8	0.9
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	11	0.9
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	8	0.9
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	8	0.9
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	8	0.9
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	8	0.9
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	8	0.9
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	8	0.9
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	8	0.9
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	8	0.9
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	8	0.9
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	8	0.9
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	8	0.9
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	8	0.9
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	9	0.9
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	9	0.9
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	9	0.9
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	14	0.89
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	14	0.89
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	14	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	10	0.89
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	10	0.89
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	10	0.89
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	10	0.89
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	10	0.89
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	10	0.89
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	10	0.89
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	10	0.89
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	10	0.89
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	14	0.89
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	14	0.89
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	14	0.89
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	10	0.89
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	10	0.89
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	10	0.89
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	10	0.89
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	10	0.89
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	10	0.89
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	10	0.89
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	10	0.89
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	10	0.89
(3,502)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	13	0.88
(3,502)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	13	0.88
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	8	0.88
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	8	0.88
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	9	0.88
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	9	0.88
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	9	0.88
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	9	0.88
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	9	0.88
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	9	0.88
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	9	0.88
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	9	0.88
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	9	0.88
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	9	0.88
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	9	0.88
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	9	0.88
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	2	0.88
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	2	0.88
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	2	0.88
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	4	0.87
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	4	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,174)	1:692:A:LEU:HD11	1:696:A:ARG:HH22	2	0.87
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	4	0.86
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	11	0.86
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	11	0.86
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	11	0.86
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	14	0.86
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	14	0.86
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	11	0.86
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	11	0.86
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	11	0.86
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	0.86
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	0.86
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	0.86
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	0.86
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	0.86
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	0.86
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	0.86
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	0.86
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	0.86
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	0.86
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	0.86
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	0.86
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	0.86
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	0.86
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	0.86
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	0.86
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	0.86
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	0.86
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	13	0.86
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	13	0.86
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	13	0.86
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	13	0.86
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	13	0.86
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	13	0.86
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	13	0.86
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	13	0.86
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	13	0.86
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	4	0.85
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	4	0.85
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	4	0.85
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	4	0.85
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	4	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	4	0.85
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	4	0.85
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	4	0.85
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	4	0.85
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	4	0.85
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	4	0.85
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	4	0.85
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	6	0.85
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	6	0.85
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	6	0.85
(3,558)	1:705:A:VAL:HG11	1:702:A:LEU:HA	4	0.84
(3,558)	1:705:A:VAL:HG12	1:702:A:LEU:HA	4	0.84
(3,558)	1:705:A:VAL:HG13	1:702:A:LEU:HA	4	0.84
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	13	0.84
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	13	0.84
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	13	0.84
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	13	0.84
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	13	0.84
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	13	0.84
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	13	0.84
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	13	0.84
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	13	0.84
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	13	0.84
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	13	0.84
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	13	0.84
(3,345)	1:705:A:VAL:HG11	1:702:A:LEU:HA	4	0.84
(3,345)	1:705:A:VAL:HG12	1:702:A:LEU:HA	4	0.84
(3,345)	1:705:A:VAL:HG13	1:702:A:LEU:HA	4	0.84
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	9	0.83
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	9	0.83
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	9	0.83
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	9	0.83
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	9	0.83
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	9	0.83
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	9	0.83
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	9	0.83
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	9	0.83
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	2	0.83
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	2	0.83
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	2	0.83
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	2	0.83
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	2	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	2	0.83
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	2	0.83
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	2	0.83
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	2	0.83
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	2	0.83
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	2	0.83
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	2	0.83
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	12	0.83
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	12	0.83
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	12	0.83
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	12	0.83
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	12	0.83
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	12	0.83
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	12	0.83
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	12	0.83
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	12	0.83
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	12	0.83
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	12	0.83
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	12	0.83
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	9	0.83
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	9	0.83
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	9	0.83
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	9	0.83
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	9	0.83
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	9	0.83
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	9	0.83
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	9	0.83
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	9	0.83
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	14	0.82
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	14	0.82
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	14	0.82
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	14	0.82
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	14	0.82
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	14	0.82
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	14	0.82
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	14	0.82
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	14	0.82
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	6	0.82
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	6	0.82
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	6	0.82
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	6	0.82
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	6	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	6	0.82
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	6	0.82
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	6	0.82
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	6	0.82
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	6	0.82
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	6	0.82
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	6	0.82
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	6	0.82
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	6	0.82
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	6	0.82
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	6	0.82
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	6	0.82
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	6	0.82
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	1	0.82
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	1	0.82
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	5	0.81
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	5	0.81
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	5	0.81
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	5	0.81
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	5	0.81
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	5	0.81
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	12	0.8
(3,289)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	4	0.8
(3,289)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	4	0.8
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	0.8
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	0.8
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	0.8
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	0.8
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	0.8
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	0.8
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	0.8
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	0.8
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	0.8
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	0.8
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	0.8
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	0.8
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	0.8
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	0.8
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	0.8
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	0.8
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	0.8
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	14	0.8
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	14	0.8
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	14	0.8
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	14	0.8
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	14	0.8
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	14	0.8
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	14	0.8
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	14	0.8
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	14	0.8
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	6	0.79
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	6	0.79
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	11	0.78
(3,174)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	6	0.78
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	9	0.76
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	9	0.76
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	9	0.76
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	9	0.76
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	9	0.76
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	9	0.76
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	9	0.76
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	9	0.76
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	9	0.76
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	2	0.76
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	2	0.76
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	2	0.76
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	2	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	2	0.76
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	2	0.76
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	2	0.76
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	2	0.76
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	2	0.76
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	2	0.76
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	2	0.76
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	2	0.76
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	2	0.76
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	2	0.76
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	2	0.76
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	2	0.76
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	2	0.76
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	2	0.76
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	2	0.76
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	2	0.76
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	2	0.76
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	2	0.76
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	2	0.76
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	2	0.76
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	1	0.76
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	1	0.76
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	1	0.76
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	0.76
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	0.76
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	0.76
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	0.76
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB2	3	0.76
(2,3)	1:664:A:ASP:H	1:660:A:LEU:HB3	3	0.76
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	2	0.75
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	2	0.75
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	2	0.75
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	2	0.75
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	2	0.75
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	2	0.75
(3,602)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	12	0.75
(3,602)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	12	0.75
(3,602)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	12	0.75
(3,602)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	12	0.75
(3,602)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	12	0.75
(3,602)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	12	0.75
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	8	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	8	0.75
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	8	0.75
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	8	0.75
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	8	0.75
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	8	0.75
(3,389)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	12	0.75
(3,389)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	12	0.75
(3,389)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	12	0.75
(3,389)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	12	0.75
(3,389)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	12	0.75
(3,389)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	12	0.75
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD11	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD12	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD13	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD21	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD22	1:680:A:TRP:HE1	2	0.75
(2,1)	1:661:A:LEU:HD23	1:680:A:TRP:HE1	2	0.75
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	9	0.74
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	9	0.74
(3,174)	1:692:A:LEU:HD13	1:696:A:ARG:HH12	14	0.74
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	11	0.73
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	11	0.73
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	11	0.73
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	11	0.73
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	11	0.73
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	11	0.73
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	11	0.73
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	11	0.73
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	11	0.73
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	14	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	14	0.72
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	14	0.72
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	14	0.72
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	14	0.72
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	14	0.72
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	9	0.72
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	9	0.72
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	9	0.72
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	9	0.72
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	9	0.72
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	9	0.72
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	7	0.71
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	7	0.71
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	7	0.71
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	7	0.71
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	7	0.71
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	7	0.71
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	7	0.71
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	7	0.71
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	7	0.71
(3,588)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	9	0.71
(3,588)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	9	0.71
(3,588)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	9	0.71
(3,588)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	9	0.71
(3,588)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	9	0.71
(3,588)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	9	0.71
(3,588)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	9	0.71
(3,588)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	9	0.71
(3,588)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	9	0.71
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	14	0.71
(3,375)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	9	0.71
(3,375)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	9	0.71
(3,375)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	9	0.71
(3,375)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	9	0.71
(3,375)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	9	0.71
(3,375)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	9	0.71
(3,375)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	9	0.71
(3,375)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	9	0.71
(3,375)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	9	0.71
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	6	0.71
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	6	0.71
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	6	0.71
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	6	0.71
(3,269)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	6	0.71
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	10	0.71
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	10	0.71
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	10	0.71
(3,602)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	6	0.7
(3,602)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	6	0.7
(3,602)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	6	0.7
(3,602)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	6	0.7
(3,602)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	6	0.7
(3,602)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	6	0.7
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	8	0.7
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	8	0.7
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	8	0.7
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	8	0.7
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	8	0.7
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	8	0.7
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	13	0.7
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	13	0.7
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	13	0.7
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	13	0.7
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	13	0.7
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	13	0.7
(3,389)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	6	0.7
(3,389)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	6	0.7
(3,389)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	6	0.7
(3,389)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	6	0.7
(3,389)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	6	0.7
(3,389)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	6	0.7
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	6	0.69
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	6	0.69
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	6	0.69
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	6	0.69
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	6	0.69
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	6	0.69
(3,174)	1:692:A:LEU:HD11	1:696:A:ARG:HH11	5	0.69
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	3	0.68
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	3	0.68
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	3	0.68
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.68
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.68
(3,602)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	11	0.68
(3,602)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	11	0.68
(3,602)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	11	0.68
(3,602)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	11	0.68
(3,602)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	11	0.68
(3,602)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	11	0.68
(3,561)	1:705:A:VAL:HG21	1:701:A:VAL:HA	1	0.68
(3,561)	1:705:A:VAL:HG22	1:701:A:VAL:HA	1	0.68
(3,561)	1:705:A:VAL:HG23	1:701:A:VAL:HA	1	0.68
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	10	0.68
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	10	0.68
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	10	0.68
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	3	0.68
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	3	0.68
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	3	0.68
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	13	0.68
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	13	0.68
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	13	0.68
(3,389)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	11	0.68
(3,389)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	11	0.68
(3,389)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	11	0.68
(3,389)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	11	0.68
(3,389)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	11	0.68
(3,389)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	11	0.68
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	4	0.68
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	4	0.68
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	4	0.68
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	10	0.68
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	10	0.68
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	10	0.68
(3,174)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	11	0.68
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	4	0.68
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	4	0.68
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	4	0.68
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	5	0.68
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	5	0.68
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	5	0.68
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	9	0.67
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	13	0.67
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	7	0.65
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	7	0.65
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	7	0.65
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	7	0.65
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	7	0.65
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	3	0.65
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	3	0.65
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	3	0.65
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	8	0.65
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	8	0.65
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	8	0.65
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	8	0.65
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	8	0.65
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	8	0.65
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	12	0.64
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	12	0.64
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	12	0.64
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	12	0.64
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	12	0.64
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	12	0.64
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	1	0.64
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	1	0.64
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	1	0.64
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	1	0.64
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	1	0.64
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	1	0.64
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	3	0.64
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	3	0.64
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	3	0.64
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	3	0.64
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	3	0.64
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	3	0.64
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	4	0.63
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	4	0.63
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	4	0.63
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	3	0.63
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	3	0.63
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	3	0.63
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	3	0.63
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	3	0.63
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	3	0.63
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	8	0.63
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	8	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	8	0.63
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	8	0.63
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	8	0.63
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	8	0.63
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	8	0.63
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	8	0.63
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	8	0.63
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	10	0.63
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	12	0.63
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	14	0.63
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.63
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.63
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.63
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.63
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.63
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.63
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	4	0.63
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	4	0.63
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	4	0.63
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	8	0.63
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	8	0.63
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	8	0.63
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	8	0.63
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	8	0.63
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	8	0.63
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	8	0.63
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	8	0.63
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	8	0.63
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	4	0.62
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	4	0.62
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	4	0.62
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	4	0.62
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	4	0.62
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	4	0.62
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	11	0.62
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	11	0.62
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	11	0.62
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	11	0.62
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	11	0.62
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	11	0.62
(3,561)	1:705:A:VAL:HG21	1:701:A:VAL:HA	4	0.61
(3,561)	1:705:A:VAL:HG22	1:701:A:VAL:HA	4	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,561)	1:705:A:VAL:HG23	1:701:A:VAL:HA	4	0.61
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.61
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.61
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.61
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	14	0.61
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	14	0.61
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	14	0.61
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.61
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.61
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.61
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.61
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.61
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.61
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.61
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.61
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.61
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	14	0.61
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	14	0.61
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	14	0.61
(3,174)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	13	0.61
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	8	0.6
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	8	0.6
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	8	0.6
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	10	0.6
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	10	0.6
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	10	0.6
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	5	0.6
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	5	0.6
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	5	0.6
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	5	0.6
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	5	0.6
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	5	0.6
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	5	0.6
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	5	0.6
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	5	0.6
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	8	0.6
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	8	0.6
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	8	0.6
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.6
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.6
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.6
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.6
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.6
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	8	0.6
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	8	0.6
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	8	0.6
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	10	0.6
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	10	0.6
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	10	0.6
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	5	0.6
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	5	0.6
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	5	0.6
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	5	0.6
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	5	0.6
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	5	0.6
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	5	0.6
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	5	0.6
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	5	0.6
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	8	0.6
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	8	0.6
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	8	0.6
(3,174)	1:692:A:LEU:HD13	1:696:A:ARG:HH11	7	0.6
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	1	0.59
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	1	0.59
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	1	0.59
(3,597)	1:692:A:LEU:HD11	1:689:A:VAL:HA	2	0.59
(3,597)	1:692:A:LEU:HD12	1:689:A:VAL:HA	2	0.59
(3,597)	1:692:A:LEU:HD13	1:689:A:VAL:HA	2	0.59
(3,597)	1:692:A:LEU:HD11	1:689:A:VAL:HA	14	0.59
(3,597)	1:692:A:LEU:HD12	1:689:A:VAL:HA	14	0.59
(3,597)	1:692:A:LEU:HD13	1:689:A:VAL:HA	14	0.59
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	2	0.59
(3,561)	1:705:A:VAL:HG21	1:701:A:VAL:HA	3	0.59
(3,561)	1:705:A:VAL:HG22	1:701:A:VAL:HA	3	0.59
(3,561)	1:705:A:VAL:HG23	1:701:A:VAL:HA	3	0.59
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	6	0.59
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	6	0.59
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	6	0.59
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	6	0.59
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	6	0.59
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	6	0.59
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	12	0.59
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	12	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	12	0.59
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	12	0.59
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	12	0.59
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	12	0.59
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	5	0.59
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	5	0.59
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	5	0.59
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	1	0.59
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	1	0.59
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	1	0.59
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	5	0.58
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	6	0.58
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	9	0.58
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	9	0.58
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	9	0.58
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	10	0.58
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	10	0.58
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	10	0.58
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	10	0.58
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	10	0.58
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	10	0.58
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	10	0.58
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	10	0.58
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	3	0.58
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	3	0.58
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	3	0.58
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	3	0.58
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	3	0.58
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	3	0.58
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	9	0.58
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	9	0.58
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	9	0.58
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	5	0.58
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	5	0.58
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	5	0.58
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	5	0.58
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	5	0.58
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	5	0.58
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	8	0.57
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	2	0.57
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	2	0.57
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	2	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	2	0.57
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	2	0.57
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	2	0.57
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	2	0.57
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	2	0.57
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	2	0.57
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	5	0.57
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	3	0.57
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	3	0.57
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	3	0.57
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	12	0.57
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	12	0.57
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	12	0.57
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	14	0.57
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	14	0.57
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	14	0.57
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	5	0.57
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	5	0.57
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	5	0.57
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	5	0.57
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	5	0.57
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	5	0.57
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	3	0.57
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	3	0.57
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	3	0.57
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	12	0.57
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	12	0.57
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	12	0.57
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	0.57
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	0.57
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	0.57
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	0.57
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	0.57
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	0.57
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	0.57
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	0.57
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	0.57
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	0.57
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	0.57
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	0.57
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	0.57
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	0.57
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	0.57
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	0.57
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	0.57
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	9	0.57
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	9	0.57
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	9	0.57
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	9	0.57
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	9	0.57
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	9	0.57
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	9	0.57
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	9	0.57
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	9	0.57
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	11	0.56
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	11	0.56
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	11	0.56
(3,597)	1:692:A:LEU:HD11	1:689:A:VAL:HA	3	0.56
(3,597)	1:692:A:LEU:HD12	1:689:A:VAL:HA	3	0.56
(3,597)	1:692:A:LEU:HD13	1:689:A:VAL:HA	3	0.56
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	2	0.56
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	2	0.56
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	2	0.56
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	2	0.56
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	2	0.56
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	11	0.56
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	11	0.56
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	11	0.56
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	0.56
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	0.56
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	0.56
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	0.56
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	0.56
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	0.56
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	0.56
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	0.56
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	0.56
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	0.56
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	0.56
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	0.56
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	0.56
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	0.56
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	0.56
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	0.56
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	0.56
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	4	0.56
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	4	0.56
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	4	0.56
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	4	0.56
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	4	0.56
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	4	0.56
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	4	0.56
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	4	0.56
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	4	0.56
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	11	0.55
(3,597)	1:692:A:LEU:HD11	1:689:A:VAL:HA	4	0.55
(3,597)	1:692:A:LEU:HD12	1:689:A:VAL:HA	4	0.55
(3,597)	1:692:A:LEU:HD13	1:689:A:VAL:HA	4	0.55
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	5	0.55
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	5	0.55
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	5	0.55
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	5	0.55
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	5	0.55
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	5	0.55
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	1	0.55
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	1	0.55
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	1	0.55
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	4	0.55
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	4	0.55
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	4	0.55
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	12	0.55
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	12	0.55
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	12	0.55
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	13	0.55
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	13	0.55
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	13	0.55
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	1	0.55
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	1	0.55
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	1	0.55
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	1	0.55
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	1	0.55
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	1	0.55
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	1	0.54
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	1	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	1	0.54
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	1	0.54
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	1	0.54
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	1	0.54
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	3	0.54
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	3	0.54
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	3	0.54
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	3	0.54
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	3	0.54
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	3	0.54
(3,551)	1:704:A:LEU:HD11	1:707:A:ARG:HE	12	0.54
(3,551)	1:704:A:LEU:HD12	1:707:A:ARG:HE	12	0.54
(3,551)	1:704:A:LEU:HD13	1:707:A:ARG:HE	12	0.54
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.54
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.54
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.54
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.54
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.54
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.54
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	6	0.54
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	6	0.54
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	6	0.54
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	6	0.54
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	6	0.54
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	6	0.54
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	13	0.54
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	13	0.54
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	13	0.53
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	13	0.53
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	13	0.53
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	13	0.53
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	13	0.53
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	13	0.53
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	5	0.53
(3,597)	1:692:A:LEU:HD11	1:689:A:VAL:HA	13	0.53
(3,597)	1:692:A:LEU:HD12	1:689:A:VAL:HA	13	0.53
(3,597)	1:692:A:LEU:HD13	1:689:A:VAL:HA	13	0.53
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	3	0.53
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	10	0.53
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	5	0.53
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	5	0.53
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	1	0.53
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	1	0.53
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	1	0.53
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	1	0.53
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	1	0.53
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	1	0.53
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	8	0.53
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	8	0.53
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	8	0.53
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	11	0.53
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	11	0.53
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	11	0.53
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	11	0.53
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	11	0.53
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	11	0.53
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	5	0.53
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	5	0.53
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	5	0.53
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.53
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.53
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.53
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.53
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.53
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.53
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	3	0.52
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	3	0.52
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	3	0.52
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	3	0.52
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	3	0.52
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	3	0.52
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	4	0.52
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	4	0.52
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	4	0.52
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	4	0.52
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	4	0.52
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	4	0.52
(3,597)	1:692:A:LEU:HD11	1:689:A:VAL:HA	10	0.52
(3,597)	1:692:A:LEU:HD12	1:689:A:VAL:HA	10	0.52
(3,597)	1:692:A:LEU:HD13	1:689:A:VAL:HA	10	0.52
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	12	0.52
(3,561)	1:705:A:VAL:HG21	1:701:A:VAL:HA	8	0.52
(3,561)	1:705:A:VAL:HG22	1:701:A:VAL:HA	8	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,561)	1:705:A:VAL:HG23	1:701:A:VAL:HA	8	0.52
(3,551)	1:704:A:LEU:HD11	1:707:A:ARG:HE	14	0.52
(3,551)	1:704:A:LEU:HD12	1:707:A:ARG:HE	14	0.52
(3,551)	1:704:A:LEU:HD13	1:707:A:ARG:HE	14	0.52
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	7	0.52
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	7	0.52
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	7	0.52
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	4	0.52
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	4	0.52
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	4	0.52
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	4	0.52
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	4	0.52
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	4	0.52
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	7	0.52
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	7	0.52
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	7	0.52
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	7	0.52
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	7	0.52
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	7	0.52
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	12	0.52
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	12	0.52
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	7	0.52
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	7	0.52
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	7	0.52
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	12	0.51
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	12	0.51
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	12	0.51
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	12	0.51
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	12	0.51
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	12	0.51
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	6	0.51
(3,551)	1:704:A:LEU:HD11	1:707:A:ARG:HE	6	0.51
(3,551)	1:704:A:LEU:HD12	1:707:A:ARG:HE	6	0.51
(3,551)	1:704:A:LEU:HD13	1:707:A:ARG:HE	6	0.51
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	3	0.51
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	3	0.51
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	3	0.51
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.51
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.51
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.51
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.51
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.51
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	10	0.5
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	10	0.5
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	10	0.5
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	10	0.5
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	10	0.5
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	10	0.5
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	3	0.5
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	3	0.5
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	3	0.5
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	3	0.5
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	3	0.5
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	3	0.5
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	3	0.5
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	3	0.5
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	3	0.5
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	10	0.5
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	4	0.5
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	4	0.5
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	4	0.5
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	4	0.5
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	4	0.5
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	4	0.5
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	7	0.5
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	7	0.5
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	7	0.5
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	3	0.5
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	3	0.5
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	3	0.5
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	3	0.5
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	3	0.5
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	3	0.5
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	3	0.5
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	3	0.5
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	3	0.5
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD11	7	0.5
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD12	7	0.5
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD13	7	0.5
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD21	7	0.5
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD22	7	0.5
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD23	7	0.5
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.5
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.5
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.5
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.5
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.5
(3,638)	1:701:A:VAL:HG11	1:698:A:VAL:HA	3	0.49
(3,638)	1:701:A:VAL:HG12	1:698:A:VAL:HA	3	0.49
(3,638)	1:701:A:VAL:HG13	1:698:A:VAL:HA	3	0.49
(3,638)	1:701:A:VAL:HG21	1:698:A:VAL:HA	3	0.49
(3,638)	1:701:A:VAL:HG22	1:698:A:VAL:HA	3	0.49
(3,638)	1:701:A:VAL:HG23	1:698:A:VAL:HA	3	0.49
(3,638)	1:701:A:VAL:HG11	1:698:A:VAL:HA	12	0.49
(3,638)	1:701:A:VAL:HG12	1:698:A:VAL:HA	12	0.49
(3,638)	1:701:A:VAL:HG13	1:698:A:VAL:HA	12	0.49
(3,638)	1:701:A:VAL:HG21	1:698:A:VAL:HA	12	0.49
(3,638)	1:701:A:VAL:HG22	1:698:A:VAL:HA	12	0.49
(3,638)	1:701:A:VAL:HG23	1:698:A:VAL:HA	12	0.49
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	9	0.49
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	5	0.49
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	3	0.49
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	3	0.49
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	3	0.49
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	3	0.49
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	3	0.49
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	3	0.49
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	3	0.49
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	3	0.49
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	3	0.49
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	3	0.49
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	3	0.49
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	3	0.49
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	1	0.49
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	1	0.49
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	1	0.49
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	1	0.49
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	1	0.49
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	1	0.49
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	5	0.49
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	5	0.49
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	9	0.49
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	9	0.49
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	6	0.49
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	6	0.49
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	6	0.49
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	6	0.49
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	6	0.49
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	12	0.49
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	12	0.49
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	12	0.49
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	12	0.49
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	12	0.49
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	12	0.49
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	13	0.49
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	13	0.49
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	13	0.49
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	10	0.48
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	10	0.48
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	10	0.48
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	10	0.48
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	10	0.48
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	10	0.48
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	8	0.48
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	8	0.48
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	8	0.48
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	5	0.48
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	5	0.48
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	5	0.48
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	5	0.48
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	5	0.48
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	5	0.48
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	9	0.48
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	9	0.48
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	9	0.48
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	11	0.48
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	11	0.48
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	11	0.48
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	8	0.48
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	8	0.48
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	8	0.48
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	8	0.48
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	8	0.48
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	10	0.48
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	10	0.48
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	10	0.48
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	10	0.48
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	10	0.48
(3,621)	1:698:A:VAL:HG11	1:695:A:LEU:HA	5	0.47
(3,621)	1:698:A:VAL:HG12	1:695:A:LEU:HA	5	0.47
(3,621)	1:698:A:VAL:HG13	1:695:A:LEU:HA	5	0.47
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	14	0.47
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	14	0.47
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	14	0.47
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	14	0.47
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	14	0.47
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	14	0.47
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	11	0.47
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	11	0.47
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	11	0.47
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	11	0.47
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	11	0.47
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	11	0.47
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	12	0.47
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	12	0.47
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	12	0.47
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	12	0.47
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	12	0.47
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	12	0.47
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	5	0.47
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	5	0.47
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	5	0.47
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	4	0.47
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	2	0.47
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	2	0.47
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	2	0.47
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	3	0.47
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	3	0.47
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	3	0.47
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	3	0.47
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	3	0.47
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	3	0.47
(3,408)	1:698:A:VAL:HG11	1:695:A:LEU:HA	5	0.47
(3,408)	1:698:A:VAL:HG12	1:695:A:LEU:HA	5	0.47
(3,408)	1:698:A:VAL:HG13	1:695:A:LEU:HA	5	0.47
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	5	0.47
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	5	0.47
(3,349)	1:705:A:VAL:HG21	1:702:A:LEU:HG	14	0.47
(3,349)	1:705:A:VAL:HG22	1:702:A:LEU:HG	14	0.47
(3,349)	1:705:A:VAL:HG23	1:702:A:LEU:HG	14	0.47
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	6	0.47
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	6	0.47
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	2	0.47
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	2	0.47
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	2	0.47
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	8	0.47
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	8	0.47
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	8	0.47
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	8	0.47
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	8	0.47
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	8	0.47
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	0.47
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	0.47
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	0.47
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	0.47
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	0.47
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	0.47
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	14	0.47
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	14	0.47
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	14	0.47
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	0.47
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	0.47
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	0.47
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	0.47
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	0.47
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	0.47
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	14	0.47
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	14	0.47
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	14	0.47
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	6	0.46
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	6	0.46
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	6	0.46
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	6	0.46
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	6	0.46
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	6	0.46
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	5	0.46
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	5	0.46
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	5	0.46
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	5	0.46
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	5	0.46
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	3	0.46
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	3	0.46
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	3	0.46
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	3	0.46
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	3	0.46
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	3	0.46
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	3	0.46
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	3	0.46
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	3	0.46
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	13	0.46
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	6	0.46
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	6	0.46
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	6	0.46
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	1	0.46
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	1	0.46
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	4	0.46
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	4	0.46
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	14	0.46
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	14	0.46
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	7	0.45
(3,614)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	7	0.45
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	7	0.45
(3,614)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	7	0.45
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	7	0.45
(3,614)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	7	0.45
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	3	0.45
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	6	0.45
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	6	0.45
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	6	0.45
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	6	0.45
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	6	0.45
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	6	0.45
(3,551)	1:704:A:LEU:HD11	1:707:A:ARG:HE	3	0.45
(3,551)	1:704:A:LEU:HD12	1:707:A:ARG:HE	3	0.45
(3,551)	1:704:A:LEU:HD13	1:707:A:ARG:HE	3	0.45
(3,484)	1:673:A:PHE:H	1:672:A:TRP:H	11	0.45
(3,481)	1:672:A:TRP:H	1:673:A:PHE:H	11	0.45
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD11	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD12	9	0.45
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD13	9	0.45
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD21	9	0.45
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD22	9	0.45
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD23	9	0.45
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	11	0.45
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	11	0.45
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	14	0.45
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	14	0.45
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	14	0.45
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	14	0.45
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	14	0.45
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	14	0.45
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	0.45
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	0.45
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	0.45
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	0.45
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	0.45
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	0.45
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	0.45
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	0.45
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	0.45
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	0.45
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	0.45
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	0.45
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	0.45
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	0.45
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	0.45
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	0.45
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	0.45
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	0.45
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	8	0.45
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	8	0.45
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	8	0.45
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	8	0.45
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	8	0.45
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	8	0.45
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	8	0.45
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	8	0.45
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	8	0.45
(3,638)	1:701:A:VAL:HG11	1:698:A:VAL:HA	10	0.44
(3,638)	1:701:A:VAL:HG12	1:698:A:VAL:HA	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,638)	1:701:A:VAL:HG13	1:698:A:VAL:HA	10	0.44
(3,638)	1:701:A:VAL:HG21	1:698:A:VAL:HA	10	0.44
(3,638)	1:701:A:VAL:HG22	1:698:A:VAL:HA	10	0.44
(3,638)	1:701:A:VAL:HG23	1:698:A:VAL:HA	10	0.44
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	9	0.44
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	2	0.44
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	2	0.44
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	7	0.44
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	7	0.44
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	10	0.44
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	10	0.44
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.44
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.44
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.44
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.44
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.44
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	4	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	4	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	4	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	7	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	7	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	7	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	7	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	7	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	7	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	7	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	7	0.44
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	7	0.44
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	0.44
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	0.44
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	0.44
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	0.44
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	0.44
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	0.44
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	4	0.44
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	4	0.44
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	0.44
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	0.44
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	0.44
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	0.44
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	0.44
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	0.44
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	7	0.44
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	7	0.44
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	7	0.44
(3,638)	1:701:A:VAL:HG11	1:698:A:VAL:HA	1	0.43
(3,638)	1:701:A:VAL:HG12	1:698:A:VAL:HA	1	0.43
(3,638)	1:701:A:VAL:HG13	1:698:A:VAL:HA	1	0.43
(3,638)	1:701:A:VAL:HG21	1:698:A:VAL:HA	1	0.43
(3,638)	1:701:A:VAL:HG22	1:698:A:VAL:HA	1	0.43
(3,638)	1:701:A:VAL:HG23	1:698:A:VAL:HA	1	0.43
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	13	0.43
(3,471)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	11	0.43
(3,471)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	11	0.43
(3,471)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	11	0.43
(3,471)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	11	0.43
(3,471)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	11	0.43
(3,471)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	11	0.43
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB3	3	0.43
(3,335)	1:704:A:LEU:H	1:704:A:LEU:HB2	3	0.43
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	1	0.43
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	1	0.43
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	1	0.43
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	1	0.43
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	1	0.43
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	1	0.43
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	14	0.42
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	12	0.42
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	12	0.42
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	12	0.42
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	12	0.42
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	12	0.42
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	12	0.42
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	0.42
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	0.42
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	0.42
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	0.42
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	0.42
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	1	0.42
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	1	0.42
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	1	0.42
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	0.42
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	0.42
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	0.42
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	0.42
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	0.42
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	0.42
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	1	0.42
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	1	0.42
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	1	0.42
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	1	0.41
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.4
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.4
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.4
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.4
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.4
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.4
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.4
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.4
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.4
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	14	0.4
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	14	0.4
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	14	0.4
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	14	0.4
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	14	0.4
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	14	0.4
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	14	0.4
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	14	0.4
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	14	0.4
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	1	0.4
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	1	0.4
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	1	0.4
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	9	0.4
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	12	0.4
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	12	0.4
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	12	0.4
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	12	0.4
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	12	0.4
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	12	0.4
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	12	0.4
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	12	0.4
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	14	0.4
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	14	0.4
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	14	0.4
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	14	0.4
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	14	0.4
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	14	0.4
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	14	0.4
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	14	0.4
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	14	0.4
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	1	0.4
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	1	0.4
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	1	0.4
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	4	0.4
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	4	0.4
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	4	0.4
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	4	0.4
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	4	0.4
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	4	0.4
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	14	0.39
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	14	0.39
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	14	0.39
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	14	0.39
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	14	0.39
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	14	0.39
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	14	0.39
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	14	0.39
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	14	0.39
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	13	0.39
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	0.39
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	0.39
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	0.39
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	0.39
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	0.39
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	0.39
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	13	0.39
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	13	0.39
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	0.39
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	0.39
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	0.39
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	0.39
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	0.39
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	0.39
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	13	0.39
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	13	0.39
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	13	0.39
(3,638)	1:701:A:VAL:HG11	1:698:A:VAL:HA	9	0.38
(3,638)	1:701:A:VAL:HG12	1:698:A:VAL:HA	9	0.38
(3,638)	1:701:A:VAL:HG13	1:698:A:VAL:HA	9	0.38
(3,638)	1:701:A:VAL:HG21	1:698:A:VAL:HA	9	0.38
(3,638)	1:701:A:VAL:HG22	1:698:A:VAL:HA	9	0.38
(3,638)	1:701:A:VAL:HG23	1:698:A:VAL:HA	9	0.38
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	1	0.38
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	6	0.38
(3,289)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	8	0.38
(3,289)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	8	0.38
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	5	0.38
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	5	0.38
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	5	0.38
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	5	0.38
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	5	0.38
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	5	0.38
(3,174)	1:692:A:LEU:HD12	1:696:A:ARG:HH21	8	0.38
(3,441)	1:665:A:LYS:H	1:662:A:GLU:HA	5	0.37
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	3	0.37
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	3	0.37
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	3	0.37
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	3	0.37
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	3	0.37
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	3	0.37
(3,228)	1:665:A:LYS:H	1:662:A:GLU:HA	5	0.37
(3,15)	1:665:A:LYS:H	1:662:A:GLU:HA	5	0.37
(3,619)	1:697:A:ILE:HG21	1:698:A:VAL:HA	1	0.36
(3,619)	1:697:A:ILE:HG22	1:698:A:VAL:HA	1	0.36
(3,619)	1:697:A:ILE:HG23	1:698:A:VAL:HA	1	0.36
(3,596)	1:690:A:GLY:H	1:691:A:SER:H	7	0.36
(3,509)	1:682:A:ILE:HD11	1:681:A:TYR:H	13	0.36
(3,509)	1:682:A:ILE:HD12	1:681:A:TYR:H	13	0.36
(3,509)	1:682:A:ILE:HD13	1:681:A:TYR:H	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,406)	1:697:A:ILE:HG21	1:698:A:VAL:HA	1	0.36
(3,406)	1:697:A:ILE:HG22	1:698:A:VAL:HA	1	0.36
(3,406)	1:697:A:ILE:HG23	1:698:A:VAL:HA	1	0.36
(3,296)	1:682:A:ILE:HD11	1:681:A:TYR:H	13	0.36
(3,296)	1:682:A:ILE:HD12	1:681:A:TYR:H	13	0.36
(3,296)	1:682:A:ILE:HD13	1:681:A:TYR:H	13	0.36
(3,193)	1:697:A:ILE:HG21	1:698:A:VAL:HA	1	0.36
(3,193)	1:697:A:ILE:HG22	1:698:A:VAL:HA	1	0.36
(3,193)	1:697:A:ILE:HG23	1:698:A:VAL:HA	1	0.36
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	13	0.36
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	13	0.36
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	13	0.36
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	9	0.36
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	9	0.36
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	9	0.36
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	12	0.35
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD11	6	0.35
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD12	6	0.35
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD13	6	0.35
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD21	6	0.35
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD22	6	0.35
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD23	6	0.35
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	2	0.35
(3,550)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	9	0.35
(3,550)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	9	0.35
(3,550)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	9	0.35
(3,550)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	9	0.35
(3,550)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	9	0.35
(3,550)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	9	0.35
(3,385)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	7	0.35
(3,385)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	7	0.35
(3,385)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	7	0.35
(3,385)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	7	0.35
(3,385)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	7	0.35
(3,385)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	7	0.35
(3,385)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	7	0.35
(3,385)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	7	0.35
(3,385)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	7	0.35
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	8	0.35
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	8	0.35
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	8	0.35
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	8	0.35
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	8	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	1	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	1	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	1	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	2	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	2	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	2	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	7	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	7	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	7	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	8	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	8	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	8	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	12	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	12	0.35
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	12	0.35
(3,619)	1:697:A:ILE:HG21	1:698:A:VAL:HA	5	0.34
(3,619)	1:697:A:ILE:HG22	1:698:A:VAL:HA	5	0.34
(3,619)	1:697:A:ILE:HG23	1:698:A:VAL:HA	5	0.34
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	2	0.34
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	2	0.34
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	2	0.34
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	2	0.34
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	2	0.34
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	2	0.34
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	3	0.34
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	3	0.34
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	3	0.34
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	7	0.34
(3,406)	1:697:A:ILE:HG21	1:698:A:VAL:HA	5	0.34
(3,406)	1:697:A:ILE:HG22	1:698:A:VAL:HA	5	0.34
(3,406)	1:697:A:ILE:HG23	1:698:A:VAL:HA	5	0.34
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	3	0.34
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	3	0.34
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	3	0.34
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	11	0.34
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	11	0.34
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	11	0.34
(3,193)	1:697:A:ILE:HG21	1:698:A:VAL:HA	5	0.34
(3,193)	1:697:A:ILE:HG22	1:698:A:VAL:HA	5	0.34
(3,193)	1:697:A:ILE:HG23	1:698:A:VAL:HA	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	10	0.34
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	10	0.34
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	10	0.34
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	10	0.34
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	10	0.34
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	10	0.34
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	10	0.34
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	10	0.34
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	10	0.34
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	0.34
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	0.34
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	0.34
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	0.34
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	0.34
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	0.34
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	10	0.34
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	10	0.34
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	10	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	3	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	3	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	3	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	4	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	4	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	4	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	5	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	5	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	5	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	6	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	6	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	6	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	9	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	9	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	9	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	10	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	10	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	10	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	11	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	11	0.34
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	11	0.34
(3,619)	1:697:A:ILE:HG21	1:698:A:VAL:HA	10	0.33
(3,619)	1:697:A:ILE:HG22	1:698:A:VAL:HA	10	0.33
(3,619)	1:697:A:ILE:HG23	1:698:A:VAL:HA	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	4	0.33
(3,597)	1:692:A:LEU:HD11	1:689:A:VAL:HA	8	0.33
(3,597)	1:692:A:LEU:HD12	1:689:A:VAL:HA	8	0.33
(3,597)	1:692:A:LEU:HD13	1:689:A:VAL:HA	8	0.33
(3,589)	1:687:A:ILE:HG21	1:691:A:SER:HG	12	0.33
(3,589)	1:687:A:ILE:HG22	1:691:A:SER:HG	12	0.33
(3,589)	1:687:A:ILE:HG23	1:691:A:SER:HG	12	0.33
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	6	0.33
(3,406)	1:697:A:ILE:HG21	1:698:A:VAL:HA	10	0.33
(3,406)	1:697:A:ILE:HG22	1:698:A:VAL:HA	10	0.33
(3,406)	1:697:A:ILE:HG23	1:698:A:VAL:HA	10	0.33
(3,376)	1:687:A:ILE:HG21	1:691:A:SER:HG	12	0.33
(3,376)	1:687:A:ILE:HG22	1:691:A:SER:HG	12	0.33
(3,376)	1:687:A:ILE:HG23	1:691:A:SER:HG	12	0.33
(3,258)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	11	0.33
(3,258)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	11	0.33
(3,258)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	11	0.33
(3,258)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	11	0.33
(3,258)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	11	0.33
(3,258)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	11	0.33
(3,193)	1:697:A:ILE:HG21	1:698:A:VAL:HA	10	0.33
(3,193)	1:697:A:ILE:HG22	1:698:A:VAL:HA	10	0.33
(3,193)	1:697:A:ILE:HG23	1:698:A:VAL:HA	10	0.33
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	6	0.33
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	0.33
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	0.33
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	0.33
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	0.33
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	0.33
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	0.33
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	3	0.33
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	3	0.33
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	3	0.33
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	7	0.33
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	7	0.33
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	7	0.33
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	7	0.33
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	7	0.33
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	7	0.33
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	0.33
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	0.33
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	0.33
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	0.33
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	0.33
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	3	0.33
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	3	0.33
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	3	0.33
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	0.33
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	0.33
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	0.33
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	0.33
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	0.33
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	0.33
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	0.33
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	0.33
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	0.33
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	0.33
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	0.33
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	0.33
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	0.33
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	0.33
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	0.33
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	0.33
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	0.33
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	0.33
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB1	7	0.33
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB2	7	0.33
(2,9)	1:702:A:LEU:HD21	1:700:A:ALA:HB3	7	0.33
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB1	7	0.33
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB2	7	0.33
(2,9)	1:702:A:LEU:HD22	1:700:A:ALA:HB3	7	0.33
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB1	7	0.33
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB2	7	0.33
(2,9)	1:702:A:LEU:HD23	1:700:A:ALA:HB3	7	0.33
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	14	0.33
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	14	0.33
(2,5)	1:666:A:TRP:HE1	1:666:A:TRP:HD1	14	0.33
(3,619)	1:697:A:ILE:HG21	1:698:A:VAL:HA	3	0.32
(3,619)	1:697:A:ILE:HG22	1:698:A:VAL:HA	3	0.32
(3,619)	1:697:A:ILE:HG23	1:698:A:VAL:HA	3	0.32
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	10	0.32
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	10	0.32
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	10	0.32
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	10	0.32
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	10	0.32
(3,551)	1:704:A:LEU:HD11	1:707:A:ARG:HE	11	0.32
(3,551)	1:704:A:LEU:HD12	1:707:A:ARG:HE	11	0.32
(3,551)	1:704:A:LEU:HD13	1:707:A:ARG:HE	11	0.32
(3,406)	1:697:A:ILE:HG21	1:698:A:VAL:HA	3	0.32
(3,406)	1:697:A:ILE:HG22	1:698:A:VAL:HA	3	0.32
(3,406)	1:697:A:ILE:HG23	1:698:A:VAL:HA	3	0.32
(3,193)	1:697:A:ILE:HG21	1:698:A:VAL:HA	3	0.32
(3,193)	1:697:A:ILE:HG22	1:698:A:VAL:HA	3	0.32
(3,193)	1:697:A:ILE:HG23	1:698:A:VAL:HA	3	0.32
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	13	0.31
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	13	0.31
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	13	0.31
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	13	0.31
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	13	0.31
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	13	0.31
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	13	0.31
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	13	0.31
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	13	0.31
(3,597)	1:692:A:LEU:HD11	1:689:A:VAL:HA	7	0.31
(3,597)	1:692:A:LEU:HD12	1:689:A:VAL:HA	7	0.31
(3,597)	1:692:A:LEU:HD13	1:689:A:VAL:HA	7	0.31
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	11	0.31
(3,349)	1:705:A:VAL:HG21	1:702:A:LEU:HG	12	0.31
(3,349)	1:705:A:VAL:HG22	1:702:A:LEU:HG	12	0.31
(3,349)	1:705:A:VAL:HG23	1:702:A:LEU:HG	12	0.31
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	14	0.31
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	11	0.31
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	0.31
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	0.31
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	0.31
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	0.31
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	0.31
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	0.31
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	11	0.31
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	11	0.31
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	11	0.31
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	0.31
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	0.31
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	0.31
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	0.31
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	0.31
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	11	0.31
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	11	0.31
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	11	0.31
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	7	0.31
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	7	0.31
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	7	0.31
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	4	0.3
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	4	0.3
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	4	0.3
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	4	0.3
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	4	0.3
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	4	0.3
(3,504)	1:681:A:TYR:H	1:680:A:TRP:H	10	0.3
(3,499)	1:678:A:TRP:HE1	1:682:A:ILE:H	14	0.3
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD2	2	0.3
(3,337)	1:704:A:LEU:HD11	1:707:A:ARG:HD3	2	0.3
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD2	2	0.3
(3,337)	1:704:A:LEU:HD12	1:707:A:ARG:HD3	2	0.3
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD2	2	0.3
(3,337)	1:704:A:LEU:HD13	1:707:A:ARG:HD3	2	0.3
(3,291)	1:681:A:TYR:H	1:680:A:TRP:H	10	0.3
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	8	0.3
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	8	0.3
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	8	0.3
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	8	0.3
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	8	0.3
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	8	0.3
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	8	0.3
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	8	0.3
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	8	0.3
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	8	0.3
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	8	0.3
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	8	0.3
(3,78)	1:681:A:TYR:H	1:680:A:TRP:H	10	0.3
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	14	0.3
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	8	0.29
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	8	0.29
(3,620)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	8	0.29
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	8	0.29
(3,620)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	8	0.29
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	8	0.29
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	8	0.29
(3,620)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	8	0.29
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	3	0.29
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.29
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.29
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	2	0.29
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	3	0.29
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.29
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.29
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	3	0.29
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD2	13	0.29
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD3	13	0.29
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	14	0.28
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	6	0.28
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	11	0.28
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	11	0.28
(3,590)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	11	0.28
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	11	0.28
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	11	0.28
(3,590)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	11	0.28
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	11	0.28
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	11	0.28
(3,590)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	11	0.28
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	6	0.28
(3,504)	1:681:A:TYR:H	1:680:A:TRP:H	6	0.28
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	6	0.28
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD11	11	0.28
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD12	11	0.28
(3,377)	1:688:A:ILE:HD11	1:684:A:ILE:HD13	11	0.28
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD11	11	0.28
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD12	11	0.28
(3,377)	1:688:A:ILE:HD12	1:684:A:ILE:HD13	11	0.28
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD11	11	0.28
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD12	11	0.28
(3,377)	1:688:A:ILE:HD13	1:684:A:ILE:HD13	11	0.28
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	13	0.28
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	13	0.28
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	13	0.28
(3,291)	1:681:A:TYR:H	1:680:A:TRP:H	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	9	0.28
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	9	0.28
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	9	0.28
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	9	0.28
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	9	0.28
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	9	0.28
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	9	0.28
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	9	0.28
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	9	0.28
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	9	0.28
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	9	0.28
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	9	0.28
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	6	0.28
(3,78)	1:681:A:TYR:H	1:680:A:TRP:H	6	0.28
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	4	0.27
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	2	0.27
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD2	4	0.27
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD3	4	0.27
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	3	0.27
(3,570)	1:707:A:ARG:H	1:704:A:LEU:HA	7	0.27
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.27
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	4	0.27
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD2	4	0.27
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD3	4	0.27
(3,349)	1:705:A:VAL:HG21	1:702:A:LEU:HG	5	0.27
(3,349)	1:705:A:VAL:HG22	1:702:A:LEU:HG	5	0.27
(3,349)	1:705:A:VAL:HG23	1:702:A:LEU:HG	5	0.27
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.27
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	14	0.27
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	14	0.27
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	14	0.27
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	14	0.27
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	14	0.27
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	14	0.27
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	4	0.27
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD2	4	0.27
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD3	4	0.27
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	9	0.27
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	5	0.27
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	0.27
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	0.27
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	0.27
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	0.27
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	0.27
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	2	0.27
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	2	0.27
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	2	0.27
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	0.27
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	0.27
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	0.27
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	0.27
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	0.27
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	0.27
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	2	0.27
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	2	0.27
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	2	0.27
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	7	0.26
(3,609)	1:695:A:LEU:H	1:694:A:GLY:H	10	0.26
(3,565)	1:706:A:ASN:H	1:704:A:LEU:H	4	0.26
(3,543)	1:704:A:LEU:H	1:701:A:VAL:HA	10	0.26
(3,499)	1:678:A:TRP:HE1	1:682:A:ILE:H	8	0.26
(3,466)	1:669:A:LEU:H	1:666:A:TRP:HA	6	0.26
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	7	0.26
(3,349)	1:705:A:VAL:HG21	1:702:A:LEU:HG	13	0.26
(3,349)	1:705:A:VAL:HG22	1:702:A:LEU:HG	13	0.26
(3,349)	1:705:A:VAL:HG23	1:702:A:LEU:HG	13	0.26
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	9	0.26
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	9	0.26
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	9	0.26
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	10	0.26
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	10	0.26
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	10	0.26
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	10	0.26
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	10	0.26
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	10	0.26
(3,253)	1:669:A:LEU:H	1:666:A:TRP:HA	6	0.26
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	9	0.26
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	9	0.26
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	9	0.26
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	9	0.26
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	9	0.26
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	9	0.26
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	4	0.26
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	8	0.26
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	10	0.26
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	10	0.26
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	10	0.26
(3,40)	1:669:A:LEU:H	1:666:A:TRP:HA	6	0.26
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	0.26
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	0.26
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	0.26
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	0.26
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	0.26
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	0.26
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	8	0.26
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	8	0.26
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	8	0.26
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	0.26
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	0.26
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	0.26
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	0.26
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	0.26
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	0.26
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	8	0.26
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	8	0.26
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	8	0.26
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	1	0.25
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	3	0.25
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	11	0.25
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	11	0.25
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	11	0.25
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	11	0.25
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	11	0.25
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	11	0.25
(3,543)	1:704:A:LEU:H	1:701:A:VAL:HA	5	0.25
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	1	0.25
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	3	0.25
(3,499)	1:678:A:TRP:HE1	1:682:A:ILE:H	12	0.25
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	1	0.25
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	3	0.25
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	4	0.25
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	4	0.25
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	4	0.25
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	4	0.25
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	4	0.25
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	4	0.25
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	4	0.25
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	4	0.25
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	4	0.25
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	4	0.25
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	4	0.25
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	4	0.25
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	4	0.25
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	4	0.25
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	4	0.25
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	4	0.25
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	4	0.25
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	1	0.25
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	3	0.25
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	3	0.25
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	11	0.25
(3,80)	1:682:A:ILE:HG21	1:679:A:LEU:H	8	0.25
(3,80)	1:682:A:ILE:HG22	1:679:A:LEU:H	8	0.25
(3,80)	1:682:A:ILE:HG23	1:679:A:LEU:H	8	0.25
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	12	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	4	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	4	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA2	13	0.25
(2,24)	1:696:A:ARG:HE	1:694:A:GLY:HA3	13	0.25
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	0.25
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	0.25
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	0.25
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	0.25
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	0.25
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	0.25
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	5	0.25
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	5	0.25
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	0.25
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	0.25
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	0.25
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	0.25
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	0.25
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	0.25
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	5	0.25
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	5	0.25
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	5	0.25
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	8	0.24
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	9	0.24
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	10	0.24
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	12	0.24
(3,588)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	6	0.24
(3,588)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	6	0.24
(3,588)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	6	0.24
(3,588)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	6	0.24
(3,588)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	6	0.24
(3,588)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	6	0.24
(3,588)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	6	0.24
(3,588)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	6	0.24
(3,588)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	6	0.24
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	6	0.24
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.24
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	8	0.24
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	9	0.24
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	10	0.24
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	12	0.24
(3,375)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	6	0.24
(3,375)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	6	0.24
(3,375)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	6	0.24
(3,375)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	6	0.24
(3,375)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	6	0.24
(3,375)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	6	0.24
(3,375)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	6	0.24
(3,375)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	6	0.24
(3,375)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	6	0.24
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.24
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	13	0.24
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	13	0.24
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	13	0.24
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	13	0.24
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	13	0.24
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	13	0.24
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	13	0.24
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	13	0.24
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	13	0.24
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	13	0.24
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	13	0.24
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	8	0.24
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	9	0.24
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	10	0.24
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	12	0.24
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	13	0.24
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	9	0.24
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	9	0.24
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	9	0.24
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	9	0.24
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	9	0.24
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	9	0.24
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.23
(3,599)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.23
(3,599)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.23
(3,599)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.23
(3,599)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.23
(3,599)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.23
(3,599)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.23
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	8	0.23
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	8	0.23
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	8	0.23
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	8	0.23
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	8	0.23
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	8	0.23
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD11	11	0.23
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD12	11	0.23
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD13	11	0.23
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD21	11	0.23
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD22	11	0.23
(3,578)	1:707:A:ARG:HE	1:704:A:LEU:HD23	11	0.23
(3,562)	1:705:A:VAL:HG21	1:702:A:LEU:HG	3	0.23
(3,562)	1:705:A:VAL:HG22	1:702:A:LEU:HG	3	0.23
(3,562)	1:705:A:VAL:HG23	1:702:A:LEU:HG	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.23
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.23
(3,386)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.23
(3,386)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.23
(3,386)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.23
(3,386)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.23
(3,386)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.23
(3,386)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.23
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	6	0.23
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	6	0.23
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	6	0.23
(3,288)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	14	0.23
(3,288)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	14	0.23
(3,288)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	14	0.23
(3,288)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	14	0.23
(3,288)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	14	0.23
(3,288)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	14	0.23
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	9	0.23
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	9	0.23
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	9	0.23
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.23
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	2	0.23
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	2	0.23
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	2	0.23
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	2	0.23
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	2	0.23
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	2	0.23
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	2	0.23
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	2	0.23
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	2	0.23
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	2	0.23
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	2	0.23
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	2	0.23
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	12	0.23
(3,214)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	12	0.23
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	12	0.23
(3,214)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	12	0.23
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	12	0.23
(3,214)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	12	0.23
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	12	0.23
(3,214)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	12	0.23
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,214)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	12	0.23
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	12	0.23
(3,214)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	12	0.23
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	2	0.23
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	3	0.23
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	3	0.23
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	3	0.23
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	3	0.23
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	3	0.23
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	3	0.23
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	1	0.23
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	1	0.23
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	1	0.23
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	1	0.23
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	1	0.23
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	1	0.23
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	2	0.23
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	2	0.23
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	2	0.23
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	2	0.23
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	2	0.23
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	2	0.23
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	13	0.23
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	13	0.23
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	13	0.23
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	13	0.23
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	13	0.23
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	13	0.23
(3,173)	1:692:A:LEU:HD11	1:691:A:SER:HB2	11	0.23
(3,173)	1:692:A:LEU:HD11	1:691:A:SER:HB3	11	0.23
(3,173)	1:692:A:LEU:HD12	1:691:A:SER:HB2	11	0.23
(3,173)	1:692:A:LEU:HD12	1:691:A:SER:HB3	11	0.23
(3,173)	1:692:A:LEU:HD13	1:691:A:SER:HB2	11	0.23
(3,173)	1:692:A:LEU:HD13	1:691:A:SER:HB3	11	0.23
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	6	0.23
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	1	0.23
(3,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	14	0.23
(3,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	14	0.23
(3,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	14	0.23
(3,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	14	0.23
(3,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	14	0.23
(3,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	9	0.23
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	9	0.23
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	9	0.23
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	9	0.23
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	9	0.23
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	9	0.23
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	9	0.23
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	9	0.23
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	9	0.23
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	3	0.23
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.22
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.22
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	1	0.22
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	11	0.22
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	13	0.22
(3,606)	1:693:A:ILE:HG21	1:694:A:GLY:H	11	0.22
(3,606)	1:693:A:ILE:HG22	1:694:A:GLY:H	11	0.22
(3,606)	1:693:A:ILE:HG23	1:694:A:GLY:H	11	0.22
(3,597)	1:692:A:LEU:HD11	1:689:A:VAL:HA	1	0.22
(3,597)	1:692:A:LEU:HD12	1:689:A:VAL:HA	1	0.22
(3,597)	1:692:A:LEU:HD13	1:689:A:VAL:HA	1	0.22
(3,597)	1:692:A:LEU:HD11	1:689:A:VAL:HA	9	0.22
(3,597)	1:692:A:LEU:HD12	1:689:A:VAL:HA	9	0.22
(3,597)	1:692:A:LEU:HD13	1:689:A:VAL:HA	9	0.22
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	12	0.22
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD1	9	0.22
(3,593)	1:689:A:VAL:HG21	1:685:A:PHE:HD2	9	0.22
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD1	9	0.22
(3,593)	1:689:A:VAL:HG22	1:685:A:PHE:HD2	9	0.22
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD1	9	0.22
(3,593)	1:689:A:VAL:HG23	1:685:A:PHE:HD2	9	0.22
(3,576)	1:707:A:ARG:H	1:707:A:ARG:HG2	8	0.22
(3,576)	1:707:A:ARG:H	1:707:A:ARG:HG3	8	0.22
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	1	0.22
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	1	0.22
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	1	0.22
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	1	0.22
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	1	0.22
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	1	0.22
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	12	0.22
(3,510)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	5	0.22
(3,510)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,510)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	5	0.22
(3,510)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	5	0.22
(3,510)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	5	0.22
(3,510)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	5	0.22
(3,499)	1:678:A:TRP:HE1	1:682:A:ILE:H	5	0.22
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	9	0.22
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	9	0.22
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	9	0.22
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	9	0.22
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	9	0.22
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	9	0.22
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.22
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.22
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.22
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	1	0.22
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	11	0.22
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	13	0.22
(3,393)	1:693:A:ILE:HG21	1:694:A:GLY:H	11	0.22
(3,393)	1:693:A:ILE:HG22	1:694:A:GLY:H	11	0.22
(3,393)	1:693:A:ILE:HG23	1:694:A:GLY:H	11	0.22
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	12	0.22
(3,363)	1:707:A:ARG:H	1:707:A:ARG:HG2	8	0.22
(3,363)	1:707:A:ARG:H	1:707:A:ARG:HG3	8	0.22
(3,297)	1:682:A:ILE:HD11	1:685:A:PHE:HB2	5	0.22
(3,297)	1:682:A:ILE:HD11	1:685:A:PHE:HB3	5	0.22
(3,297)	1:682:A:ILE:HD12	1:685:A:PHE:HB2	5	0.22
(3,297)	1:682:A:ILE:HD12	1:685:A:PHE:HB3	5	0.22
(3,297)	1:682:A:ILE:HD13	1:685:A:PHE:HB2	5	0.22
(3,297)	1:682:A:ILE:HD13	1:685:A:PHE:HB3	5	0.22
(3,289)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	1	0.22
(3,289)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	1	0.22
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	6	0.22
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	6	0.22
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	6	0.22
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.22
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	4	0.22
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	14	0.22
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	9	0.22
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	9	0.22
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	9	0.22
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	9	0.22
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	9	0.22
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	1	0.22
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	11	0.22
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	13	0.22
(3,180)	1:693:A:ILE:HG21	1:694:A:GLY:H	11	0.22
(3,180)	1:693:A:ILE:HG22	1:694:A:GLY:H	11	0.22
(3,180)	1:693:A:ILE:HG23	1:694:A:GLY:H	11	0.22
(3,150)	1:707:A:ARG:H	1:707:A:ARG:HG2	8	0.22
(3,150)	1:707:A:ARG:H	1:707:A:ARG:HG3	8	0.22
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	1	0.22
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	1	0.22
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	1	0.22
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	1	0.22
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	1	0.22
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	1	0.22
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	12	0.22
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	3	0.22
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	5	0.22
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	10	0.22
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	5	0.22
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	6	0.22
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	6	0.22
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	6	0.22
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	12	0.22
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	0.22
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	0.22
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	0.22
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	0.22
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	0.22
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	0.22
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	9	0.22
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	9	0.22
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	9	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	1	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	1	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	1	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	1	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	1	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	1	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	5	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	5	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	5	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	5	0.22
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	5	0.22
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	0.22
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	0.22
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	0.22
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	0.22
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	0.22
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	0.22
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	9	0.22
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	9	0.22
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	9	0.22
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.21
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.21
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.21
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.21
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.21
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.21
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	6	0.21
(3,606)	1:693:A:ILE:HG21	1:694:A:GLY:H	5	0.21
(3,606)	1:693:A:ILE:HG22	1:694:A:GLY:H	5	0.21
(3,606)	1:693:A:ILE:HG23	1:694:A:GLY:H	5	0.21
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	13	0.21
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	8	0.21
(3,551)	1:704:A:LEU:HD11	1:707:A:ARG:HE	4	0.21
(3,551)	1:704:A:LEU:HD12	1:707:A:ARG:HE	4	0.21
(3,551)	1:704:A:LEU:HD13	1:707:A:ARG:HE	4	0.21
(3,543)	1:704:A:LEU:H	1:701:A:VAL:HA	7	0.21
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	13	0.21
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	2	0.21
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.21
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.21
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.21
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.21
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.21
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.21
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.21
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.21
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.21
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.21
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.21
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,393)	1:693:A:ILE:HG21	1:694:A:GLY:H	5	0.21
(3,393)	1:693:A:ILE:HG22	1:694:A:GLY:H	5	0.21
(3,393)	1:693:A:ILE:HG23	1:694:A:GLY:H	5	0.21
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	13	0.21
(3,270)	1:672:A:TRP:HE1	1:671:A:ASN:H	8	0.21
(3,266)	1:671:A:ASN:H	1:672:A:TRP:HE1	8	0.21
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.21
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.21
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.21
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.21
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.21
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	1	0.21
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	3	0.21
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	6	0.21
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	9	0.21
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	10	0.21
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	13	0.21
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	1	0.21
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	1	0.21
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	1	0.21
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	1	0.21
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	1	0.21
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	1	0.21
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD1	3	0.21
(3,197)	1:698:A:VAL:HG11	1:699:A:PHE:HD2	3	0.21
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD1	3	0.21
(3,197)	1:698:A:VAL:HG12	1:699:A:PHE:HD2	3	0.21
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD1	3	0.21
(3,197)	1:698:A:VAL:HG13	1:699:A:PHE:HD2	3	0.21
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	6	0.21
(3,180)	1:693:A:ILE:HG21	1:694:A:GLY:H	5	0.21
(3,180)	1:693:A:ILE:HG22	1:694:A:GLY:H	5	0.21
(3,180)	1:693:A:ILE:HG23	1:694:A:GLY:H	5	0.21
(3,162)	1:687:A:ILE:HD11	1:684:A:ILE:HD11	9	0.21
(3,162)	1:687:A:ILE:HD11	1:684:A:ILE:HD12	9	0.21
(3,162)	1:687:A:ILE:HD11	1:684:A:ILE:HD13	9	0.21
(3,162)	1:687:A:ILE:HD12	1:684:A:ILE:HD11	9	0.21
(3,162)	1:687:A:ILE:HD12	1:684:A:ILE:HD12	9	0.21
(3,162)	1:687:A:ILE:HD12	1:684:A:ILE:HD13	9	0.21
(3,162)	1:687:A:ILE:HD13	1:684:A:ILE:HD11	9	0.21
(3,162)	1:687:A:ILE:HD13	1:684:A:ILE:HD12	9	0.21
(3,162)	1:687:A:ILE:HD13	1:684:A:ILE:HD13	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	13	0.21
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	9	0.21
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	10	0.21
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	13	0.21
(3,57)	1:672:A:TRP:HE1	1:671:A:ASN:H	8	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	14	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	14	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	14	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	14	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	14	0.21
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	14	0.21
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	2	0.21
(3,53)	1:671:A:ASN:H	1:672:A:TRP:HE1	8	0.21
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	13	0.21
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	13	0.21
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	13	0.21
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	13	0.21
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	13	0.21
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	13	0.21
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	9	0.21
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	2	0.21
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	8	0.21
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	9	0.21
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	14	0.21
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	8	0.21
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	8	0.21
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	8	0.21
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	8	0.21
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	8	0.21
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	8	0.21
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.2
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.2
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.2
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	4	0.2
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	4	0.2
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	4	0.2
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	4	0.2
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	4	0.2
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	4	0.2
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	13	0.2
(3,618)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	13	0.2
(3,618)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	13	0.2
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	13	0.2
(3,618)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	13	0.2
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.2
(3,576)	1:707:A:ARG:H	1:707:A:ARG:HG2	6	0.2
(3,576)	1:707:A:ARG:H	1:707:A:ARG:HG3	6	0.2
(3,543)	1:704:A:LEU:H	1:701:A:VAL:HA	13	0.2
(3,499)	1:678:A:TRP:HE1	1:682:A:ILE:H	6	0.2
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	10	0.2
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	13	0.2
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	14	0.2
(3,458)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.2
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.2
(3,441)	1:665:A:LYS:H	1:662:A:GLU:HA	12	0.2
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.2
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.2
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.2
(3,420)	1:700:A:ALA:HB1	1:697:A:ILE:HA	10	0.2
(3,420)	1:700:A:ALA:HB2	1:697:A:ILE:HA	10	0.2
(3,420)	1:700:A:ALA:HB3	1:697:A:ILE:HA	10	0.2
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.2
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.2
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.2
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.2
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB2	14	0.2
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB3	14	0.2
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB2	14	0.2
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB3	14	0.2
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB2	14	0.2
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB3	14	0.2
(3,363)	1:707:A:ARG:H	1:707:A:ARG:HG2	6	0.2
(3,363)	1:707:A:ARG:H	1:707:A:ARG:HG3	6	0.2
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	1	0.2
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	1	0.2
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	1	0.2
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.2
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.2
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.2
(3,245)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.2
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,228)	1:665:A:LYS:H	1:662:A:GLU:HA	12	0.2
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.2
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.2
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.2
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	5	0.2
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	7	0.2
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	8	0.2
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	11	0.2
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	14	0.2
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB2	14	0.2
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB3	14	0.2
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB2	14	0.2
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB3	14	0.2
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB2	14	0.2
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB3	14	0.2
(3,150)	1:707:A:ARG:H	1:707:A:ARG:HG2	6	0.2
(3,150)	1:707:A:ARG:H	1:707:A:ARG:HG3	6	0.2
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	12	0.2
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	14	0.2
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	7	0.2
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	12	0.2
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	6	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	1	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	1	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	1	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	11	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	11	0.2
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	11	0.2
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	10	0.2
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	13	0.2
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	14	0.2
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	2	0.2
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	2	0.2
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	2	0.2
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	2	0.2
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	2	0.2
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	2	0.2
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	5	0.2
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	1	0.2
(3,15)	1:665:A:LYS:H	1:662:A:GLU:HA	12	0.2
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	4	0.2
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	11	0.2
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	4	0.2
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	4	0.2
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	4	0.2
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	4	0.2
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	4	0.2
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	4	0.2
(3,629)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.19
(3,617)	1:696:A:ARG:H	1:696:A:ARG:HE	14	0.19
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	2	0.19
(3,599)	1:692:A:LEU:HD11	1:691:A:SER:HB2	8	0.19
(3,599)	1:692:A:LEU:HD11	1:691:A:SER:HB3	8	0.19
(3,599)	1:692:A:LEU:HD12	1:691:A:SER:HB2	8	0.19
(3,599)	1:692:A:LEU:HD12	1:691:A:SER:HB3	8	0.19
(3,599)	1:692:A:LEU:HD13	1:691:A:SER:HB2	8	0.19
(3,599)	1:692:A:LEU:HD13	1:691:A:SER:HB3	8	0.19
(3,503)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	13	0.19
(3,503)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	13	0.19
(3,503)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	13	0.19
(3,499)	1:678:A:TRP:HE1	1:682:A:ILE:H	9	0.19
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	3	0.19
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	7	0.19
(3,446)	1:665:A:LYS:H	1:666:A:TRP:HD1	14	0.19
(3,441)	1:665:A:LYS:H	1:662:A:GLU:HA	3	0.19
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.19
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	6	0.19
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.19
(3,416)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.19
(3,404)	1:696:A:ARG:H	1:696:A:ARG:HE	14	0.19
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	2	0.19
(3,386)	1:692:A:LEU:HD11	1:691:A:SER:HB2	8	0.19
(3,386)	1:692:A:LEU:HD11	1:691:A:SER:HB3	8	0.19
(3,386)	1:692:A:LEU:HD12	1:691:A:SER:HB2	8	0.19
(3,386)	1:692:A:LEU:HD12	1:691:A:SER:HB3	8	0.19
(3,386)	1:692:A:LEU:HD13	1:691:A:SER:HB2	8	0.19
(3,386)	1:692:A:LEU:HD13	1:691:A:SER:HB3	8	0.19
(3,349)	1:705:A:VAL:HG21	1:702:A:LEU:HG	9	0.19
(3,349)	1:705:A:VAL:HG22	1:702:A:LEU:HG	9	0.19
(3,349)	1:705:A:VAL:HG23	1:702:A:LEU:HG	9	0.19
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	12	0.19
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	12	0.19
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	14	0.19
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	14	0.19
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	14	0.19
(3,290)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	13	0.19
(3,290)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	13	0.19
(3,290)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	13	0.19
(3,289)	1:680:A:TRP:HE1	1:683:A:ARG:HH21	10	0.19
(3,289)	1:680:A:TRP:HE1	1:683:A:ARG:HH22	10	0.19
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	2	0.19
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	2	0.19
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	2	0.19
(3,233)	1:665:A:LYS:H	1:666:A:TRP:HD1	14	0.19
(3,228)	1:665:A:LYS:H	1:662:A:GLU:HA	3	0.19
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.19
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	6	0.19
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.19
(3,203)	1:700:A:ALA:H	1:699:A:PHE:HA	12	0.19
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	2	0.19
(3,173)	1:692:A:LEU:HD11	1:691:A:SER:HB2	8	0.19
(3,173)	1:692:A:LEU:HD11	1:691:A:SER:HB3	8	0.19
(3,173)	1:692:A:LEU:HD12	1:691:A:SER:HB2	8	0.19
(3,173)	1:692:A:LEU:HD12	1:691:A:SER:HB3	8	0.19
(3,173)	1:692:A:LEU:HD13	1:691:A:SER:HB2	8	0.19
(3,173)	1:692:A:LEU:HD13	1:691:A:SER:HB3	8	0.19
(3,132)	1:705:A:VAL:HG11	1:702:A:LEU:HA	13	0.19
(3,132)	1:705:A:VAL:HG12	1:702:A:LEU:HA	13	0.19
(3,132)	1:705:A:VAL:HG13	1:702:A:LEU:HA	13	0.19
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	6	0.19
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	12	0.19
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	2	0.19
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	6	0.19
(3,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD11	13	0.19
(3,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD12	13	0.19
(3,77)	1:680:A:TRP:HE1	1:684:A:ILE:HD13	13	0.19
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	9	0.19
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	2	0.19
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	2	0.19
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	2	0.19
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	3	0.19
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	7	0.19
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	6	0.19
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	6	0.19
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	6	0.19
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	6	0.19
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	6	0.19
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	12	0.19
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	12	0.19
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	12	0.19
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	12	0.19
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	12	0.19
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	12	0.19
(3,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	14	0.19
(3,15)	1:665:A:LYS:H	1:662:A:GLU:HA	3	0.19
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	5	0.19
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	6	0.19
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	10	0.19
(3,606)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.18
(3,606)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.18
(3,606)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.18
(3,606)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.18
(3,606)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.18
(3,606)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.18
(3,606)	1:693:A:ILE:HG21	1:694:A:GLY:H	13	0.18
(3,606)	1:693:A:ILE:HG22	1:694:A:GLY:H	13	0.18
(3,606)	1:693:A:ILE:HG23	1:694:A:GLY:H	13	0.18
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG21	9	0.18
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG22	9	0.18
(3,598)	1:692:A:LEU:HD11	1:689:A:VAL:HG23	9	0.18
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG21	9	0.18
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG22	9	0.18
(3,598)	1:692:A:LEU:HD12	1:689:A:VAL:HG23	9	0.18
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG21	9	0.18
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG22	9	0.18
(3,598)	1:692:A:LEU:HD13	1:689:A:VAL:HG23	9	0.18
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	10	0.18
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	5	0.18
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	5	0.18
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	5	0.18
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	5	0.18
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	5	0.18
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	5	0.18
(3,543)	1:704:A:LEU:H	1:701:A:VAL:HA	11	0.18
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.18
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.18
(3,393)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.18
(3,393)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.18
(3,393)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.18
(3,393)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.18
(3,393)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.18
(3,393)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.18
(3,393)	1:693:A:ILE:HG21	1:694:A:GLY:H	13	0.18
(3,393)	1:693:A:ILE:HG22	1:694:A:GLY:H	13	0.18
(3,393)	1:693:A:ILE:HG23	1:694:A:GLY:H	13	0.18
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	10	0.18
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD11	10	0.18
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD12	10	0.18
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD13	10	0.18
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD21	10	0.18
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD22	10	0.18
(3,365)	1:707:A:ARG:HE	1:704:A:LEU:HD23	10	0.18
(3,348)	1:705:A:VAL:HG21	1:701:A:VAL:HA	1	0.18
(3,348)	1:705:A:VAL:HG22	1:701:A:VAL:HA	1	0.18
(3,348)	1:705:A:VAL:HG23	1:701:A:VAL:HA	1	0.18
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	7	0.18
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	7	0.18
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	7	0.18
(3,288)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	12	0.18
(3,288)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	12	0.18
(3,288)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	12	0.18
(3,288)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	12	0.18
(3,288)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	12	0.18
(3,288)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	12	0.18
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	5	0.18
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	5	0.18
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	5	0.18
(3,259)	1:670:A:TRP:H	1:667:A:ALA:HA	2	0.18
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.18
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.18
(3,195)	1:698:A:VAL:HG11	1:695:A:LEU:HA	12	0.18
(3,195)	1:698:A:VAL:HG12	1:695:A:LEU:HA	12	0.18
(3,195)	1:698:A:VAL:HG13	1:695:A:LEU:HA	12	0.18
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	3	0.18
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	3	0.18
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	3	0.18
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	3	0.18
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	3	0.18
(3,180)	1:693:A:ILE:HG21	1:694:A:GLY:H	3	0.18
(3,180)	1:693:A:ILE:HG22	1:694:A:GLY:H	3	0.18
(3,180)	1:693:A:ILE:HG23	1:694:A:GLY:H	3	0.18
(3,180)	1:693:A:ILE:HG21	1:694:A:GLY:H	8	0.18
(3,180)	1:693:A:ILE:HG22	1:694:A:GLY:H	8	0.18
(3,180)	1:693:A:ILE:HG23	1:694:A:GLY:H	8	0.18
(3,180)	1:693:A:ILE:HG21	1:694:A:GLY:H	13	0.18
(3,180)	1:693:A:ILE:HG22	1:694:A:GLY:H	13	0.18
(3,180)	1:693:A:ILE:HG23	1:694:A:GLY:H	13	0.18
(3,177)	1:693:A:ILE:HD11	1:697:A:ILE:H	10	0.18
(3,177)	1:693:A:ILE:HD12	1:697:A:ILE:H	10	0.18
(3,177)	1:693:A:ILE:HD13	1:697:A:ILE:H	10	0.18
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	5	0.18
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	5	0.18
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	5	0.18
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	5	0.18
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	5	0.18
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	5	0.18
(3,135)	1:705:A:VAL:HG21	1:701:A:VAL:HA	1	0.18
(3,135)	1:705:A:VAL:HG22	1:701:A:VAL:HA	1	0.18
(3,135)	1:705:A:VAL:HG23	1:701:A:VAL:HA	1	0.18
(3,132)	1:705:A:VAL:HG11	1:702:A:LEU:HA	9	0.18
(3,132)	1:705:A:VAL:HG12	1:702:A:LEU:HA	9	0.18
(3,132)	1:705:A:VAL:HG13	1:702:A:LEU:HA	9	0.18
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	10	0.18
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	2	0.18
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	4	0.18
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	5	0.18
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	8	0.18
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	2	0.18
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	9	0.18
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	10	0.18
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	10	0.18
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	10	0.18
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	10	0.18
(3,75)	1:679:A:LEU:HD11	1:678:A:TRP:HH2	12	0.18
(3,75)	1:679:A:LEU:HD12	1:678:A:TRP:HH2	12	0.18
(3,75)	1:679:A:LEU:HD13	1:678:A:TRP:HH2	12	0.18
(3,75)	1:679:A:LEU:HD21	1:678:A:TRP:HH2	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,75)	1:679:A:LEU:HD22	1:678:A:TRP:HH2	12	0.18
(3,75)	1:679:A:LEU:HD23	1:678:A:TRP:HH2	12	0.18
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	5	0.18
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	5	0.18
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	5	0.18
(3,46)	1:670:A:TRP:H	1:667:A:ALA:HA	2	0.18
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	10	0.18
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	10	0.18
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	10	0.18
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	10	0.18
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	10	0.18
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	10	0.18
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	11	0.18
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	14	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	6	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	6	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	6	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	6	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	6	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	6	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	6	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	6	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	6	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD21	12	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD22	12	0.18
(2,21)	1:694:A:GLY:H	1:692:A:LEU:HD23	12	0.18
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	3	0.18
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	3	0.18
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	3	0.18
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	3	0.18
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	3	0.18
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	3	0.18
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	0.18
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	0.18
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	0.18
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	13	0.18
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	13	0.18
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	0.18
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	0.18
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	0.18
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	0.18
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	0.18
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	0.18
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	6	0.18
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	6	0.18
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	6	0.18
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	0.18
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	0.18
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	0.18
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	0.18
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	0.18
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	0.18
(2,15)	1:692:A:LEU:HD21	1:694:A:GLY:H	12	0.18
(2,15)	1:692:A:LEU:HD22	1:694:A:GLY:H	12	0.18
(2,15)	1:692:A:LEU:HD23	1:694:A:GLY:H	12	0.18
(2,11)	1:686:A:ILE:H	1:686:A:ILE:HG21	4	0.18
(2,11)	1:686:A:ILE:H	1:686:A:ILE:HG22	4	0.18
(2,11)	1:686:A:ILE:H	1:686:A:ILE:HG23	4	0.18
(2,11)	1:686:A:ILE:H	1:686:A:ILE:HG21	4	0.18
(2,11)	1:686:A:ILE:H	1:686:A:ILE:HG22	4	0.18
(2,11)	1:686:A:ILE:H	1:686:A:ILE:HG23	4	0.18
(2,11)	1:686:A:ILE:H	1:686:A:ILE:HG21	4	0.18
(2,11)	1:686:A:ILE:H	1:686:A:ILE:HG22	4	0.18
(2,11)	1:686:A:ILE:H	1:686:A:ILE:HG23	4	0.18
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	8	0.18
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	8	0.18
(1,6)	1:670:A:TRP:HE1	2:801:B:QOJ:H11	8	0.18
(3,617)	1:696:A:ARG:H	1:696:A:ARG:HE	5	0.17
(3,616)	1:696:A:ARG:H	1:695:A:LEU:H	5	0.17
(3,606)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.17
(3,606)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.17
(3,606)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.17
(3,599)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.17
(3,599)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.17
(3,599)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.17
(3,599)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.17
(3,599)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,599)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.17
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	2	0.17
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	4	0.17
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	3	0.17
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	3	0.17
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	3	0.17
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	3	0.17
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	3	0.17
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	3	0.17
(3,543)	1:704:A:LEU:H	1:701:A:VAL:HA	12	0.17
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	2	0.17
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	4	0.17
(3,520)	1:684:A:ILE:HG21	1:688:A:ILE:H	5	0.17
(3,520)	1:684:A:ILE:HG22	1:688:A:ILE:H	5	0.17
(3,520)	1:684:A:ILE:HG23	1:688:A:ILE:H	5	0.17
(3,514)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.17
(3,514)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.17
(3,514)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.17
(3,514)	1:684:A:ILE:HD11	1:681:A:TYR:HA	14	0.17
(3,514)	1:684:A:ILE:HD12	1:681:A:TYR:HA	14	0.17
(3,514)	1:684:A:ILE:HD13	1:681:A:TYR:HA	14	0.17
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	9	0.17
(3,458)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.17
(3,458)	1:667:A:ALA:H	1:666:A:TRP:HD1	13	0.17
(3,446)	1:665:A:LYS:H	1:666:A:TRP:HD1	6	0.17
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.17
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.17
(3,404)	1:696:A:ARG:H	1:696:A:ARG:HE	5	0.17
(3,403)	1:696:A:ARG:H	1:695:A:LEU:H	5	0.17
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	3	0.17
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	3	0.17
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	3	0.17
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	3	0.17
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	3	0.17
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	3	0.17
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	7	0.17
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	7	0.17
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	7	0.17
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	7	0.17
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	7	0.17
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	7	0.17
(3,393)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,393)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.17
(3,393)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.17
(3,386)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.17
(3,386)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.17
(3,386)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.17
(3,386)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.17
(3,386)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.17
(3,386)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.17
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	2	0.17
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	4	0.17
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	5	0.17
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	5	0.17
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	5	0.17
(3,302)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	2	0.17
(3,302)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	2	0.17
(3,302)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	2	0.17
(3,302)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	2	0.17
(3,302)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	2	0.17
(3,302)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	2	0.17
(3,301)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.17
(3,301)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.17
(3,301)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.17
(3,301)	1:684:A:ILE:HD11	1:681:A:TYR:HA	14	0.17
(3,301)	1:684:A:ILE:HD12	1:681:A:TYR:HA	14	0.17
(3,301)	1:684:A:ILE:HD13	1:681:A:TYR:HA	14	0.17
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	4	0.17
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	4	0.17
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	4	0.17
(3,259)	1:670:A:TRP:H	1:667:A:ALA:HA	11	0.17
(3,245)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.17
(3,245)	1:667:A:ALA:H	1:666:A:TRP:HD1	13	0.17
(3,233)	1:665:A:LYS:H	1:666:A:TRP:HD1	6	0.17
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.17
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.17
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	2	0.17
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	2	0.17
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	2	0.17
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	2	0.17
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	2	0.17
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	2	0.17
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	13	0.17
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	13	0.17
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	13	0.17
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	13	0.17
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	13	0.17
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	14	0.17
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	14	0.17
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	14	0.17
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	14	0.17
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	14	0.17
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	14	0.17
(3,190)	1:696:A:ARG:H	1:695:A:LEU:H	5	0.17
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	3	0.17
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	3	0.17
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	3	0.17
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	3	0.17
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	3	0.17
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	3	0.17
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	7	0.17
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	7	0.17
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	7	0.17
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	7	0.17
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	7	0.17
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	7	0.17
(3,180)	1:693:A:ILE:HG21	1:694:A:GLY:H	4	0.17
(3,180)	1:693:A:ILE:HG22	1:694:A:GLY:H	4	0.17
(3,180)	1:693:A:ILE:HG23	1:694:A:GLY:H	4	0.17
(3,173)	1:692:A:LEU:HD11	1:691:A:SER:HB2	5	0.17
(3,173)	1:692:A:LEU:HD11	1:691:A:SER:HB3	5	0.17
(3,173)	1:692:A:LEU:HD12	1:691:A:SER:HB2	5	0.17
(3,173)	1:692:A:LEU:HD12	1:691:A:SER:HB3	5	0.17
(3,173)	1:692:A:LEU:HD13	1:691:A:SER:HB2	5	0.17
(3,173)	1:692:A:LEU:HD13	1:691:A:SER:HB3	5	0.17
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	3	0.17
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	3	0.17
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	3	0.17
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	3	0.17
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	3	0.17
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	3	0.17
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	2	0.17
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	4	0.17
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	1	0.17
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	5	0.17
(3,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	12	0.17
(3,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	12	0.17
(3,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	12	0.17
(3,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	14	0.17
(3,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	14	0.17
(3,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	14	0.17
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	4	0.17
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	4	0.17
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	4	0.17
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	9	0.17
(3,46)	1:670:A:TRP:H	1:667:A:ALA:HA	11	0.17
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	3	0.17
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	13	0.17
(3,20)	1:665:A:LYS:H	1:666:A:TRP:HD1	6	0.17
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	4	0.17
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	10	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD11	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD12	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD13	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD21	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD22	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD23	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD11	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD12	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD13	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD21	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD22	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD23	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD11	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD12	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD13	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD21	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD22	14	0.17
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD23	14	0.17
(3,606)	1:693:A:ILE:HG21	1:694:A:GLY:H	6	0.16
(3,606)	1:693:A:ILE:HG22	1:694:A:GLY:H	6	0.16
(3,606)	1:693:A:ILE:HG23	1:694:A:GLY:H	6	0.16
(3,606)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.16
(3,606)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.16
(3,606)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.16
(3,591)	1:688:A:ILE:HG21	1:692:A:LEU:HG	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,591)	1:688:A:ILE:HG22	1:692:A:LEU:HG	14	0.16
(3,591)	1:688:A:ILE:HG23	1:692:A:LEU:HG	14	0.16
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.16
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.16
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.16
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.16
(3,564)	1:706:A:ASN:H	1:703:A:SER:HA	11	0.16
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	12	0.16
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	12	0.16
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	12	0.16
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	12	0.16
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	12	0.16
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	12	0.16
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	1	0.16
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	4	0.16
(3,460)	1:667:A:ALA:HB1	1:664:A:ASP:HA	13	0.16
(3,460)	1:667:A:ALA:HB2	1:664:A:ASP:HA	13	0.16
(3,460)	1:667:A:ALA:HB3	1:664:A:ASP:HA	13	0.16
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.16
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.16
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.16
(3,442)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.16
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.16
(3,393)	1:693:A:ILE:HG21	1:694:A:GLY:H	6	0.16
(3,393)	1:693:A:ILE:HG22	1:694:A:GLY:H	6	0.16
(3,393)	1:693:A:ILE:HG23	1:694:A:GLY:H	6	0.16
(3,393)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.16
(3,393)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.16
(3,393)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.16
(3,378)	1:688:A:ILE:HG21	1:692:A:LEU:HG	14	0.16
(3,378)	1:688:A:ILE:HG22	1:692:A:LEU:HG	14	0.16
(3,378)	1:688:A:ILE:HG23	1:692:A:LEU:HG	14	0.16
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.16
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.16
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.16
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.16
(3,259)	1:670:A:TRP:H	1:667:A:ALA:HA	7	0.16
(3,247)	1:667:A:ALA:HB1	1:664:A:ASP:HA	13	0.16
(3,247)	1:667:A:ALA:HB2	1:664:A:ASP:HA	13	0.16
(3,247)	1:667:A:ALA:HB3	1:664:A:ASP:HA	13	0.16
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.16
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.16
(3,229)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.16
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.16
(3,192)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	9	0.16
(3,192)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	9	0.16
(3,192)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	9	0.16
(3,192)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	9	0.16
(3,192)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	9	0.16
(3,192)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	9	0.16
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	1	0.16
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	1	0.16
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	1	0.16
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	1	0.16
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	1	0.16
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	1	0.16
(3,180)	1:693:A:ILE:HG21	1:694:A:GLY:H	6	0.16
(3,180)	1:693:A:ILE:HG22	1:694:A:GLY:H	6	0.16
(3,180)	1:693:A:ILE:HG23	1:694:A:GLY:H	6	0.16
(3,180)	1:693:A:ILE:HG21	1:694:A:GLY:H	7	0.16
(3,180)	1:693:A:ILE:HG22	1:694:A:GLY:H	7	0.16
(3,180)	1:693:A:ILE:HG23	1:694:A:GLY:H	7	0.16
(3,165)	1:688:A:ILE:HG21	1:692:A:LEU:HG	14	0.16
(3,165)	1:688:A:ILE:HG22	1:692:A:LEU:HG	14	0.16
(3,165)	1:688:A:ILE:HG23	1:692:A:LEU:HG	14	0.16
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD2	6	0.16
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD3	6	0.16
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD2	7	0.16
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD3	7	0.16
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	12	0.16
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	12	0.16
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	12	0.16
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	12	0.16
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	12	0.16
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	12	0.16
(3,132)	1:705:A:VAL:HG11	1:702:A:LEU:HA	11	0.16
(3,132)	1:705:A:VAL:HG12	1:702:A:LEU:HA	11	0.16
(3,132)	1:705:A:VAL:HG13	1:702:A:LEU:HA	11	0.16
(3,99)	1:687:A:ILE:H	1:688:A:ILE:H	7	0.16
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	9	0.16
(3,80)	1:682:A:ILE:HG21	1:679:A:LEU:H	7	0.16
(3,80)	1:682:A:ILE:HG22	1:679:A:LEU:H	7	0.16
(3,80)	1:682:A:ILE:HG23	1:679:A:LEU:H	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	1	0.16
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	4	0.16
(3,46)	1:670:A:TRP:H	1:667:A:ALA:HA	7	0.16
(3,34)	1:667:A:ALA:HB1	1:664:A:ASP:HA	13	0.16
(3,34)	1:667:A:ALA:HB2	1:664:A:ASP:HA	13	0.16
(3,34)	1:667:A:ALA:HB3	1:664:A:ASP:HA	13	0.16
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	2	0.16
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	6	0.16
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	7	0.16
(3,16)	1:665:A:LYS:H	1:664:A:ASP:HA	8	0.16
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	3	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD11	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD12	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD13	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD21	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD22	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD23	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD11	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD12	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD13	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD21	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD22	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD23	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD11	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD12	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD13	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD21	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD22	12	0.16
(2,10)	1:707:A:ARG:H	1:704:A:LEU:HD23	12	0.16
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	13	0.16
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	13	0.16
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	13	0.16
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	9	0.15
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	14	0.15
(3,534)	1:702:A:LEU:H	1:704:A:LEU:H	10	0.15
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	9	0.15
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	14	0.15
(3,518)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	9	0.15
(3,518)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	9	0.15
(3,518)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	9	0.15
(3,518)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	9	0.15
(3,518)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,518)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	9	0.15
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	5	0.15
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	1	0.15
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	1	0.15
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	1	0.15
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	1	0.15
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	1	0.15
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	1	0.15
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	1	0.15
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	1	0.15
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	1	0.15
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	1	0.15
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	1	0.15
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	1	0.15
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB2	2	0.15
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB3	2	0.15
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB2	2	0.15
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB3	2	0.15
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB2	2	0.15
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB3	2	0.15
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB2	9	0.15
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB3	9	0.15
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB2	9	0.15
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB3	9	0.15
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB2	9	0.15
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB3	9	0.15
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	9	0.15
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	14	0.15
(3,340)	1:705:A:VAL:H	1:702:A:LEU:HA	10	0.15
(3,321)	1:702:A:LEU:H	1:704:A:LEU:H	10	0.15
(3,259)	1:670:A:TRP:H	1:667:A:ALA:HA	6	0.15
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	4	0.15
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	4	0.15
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	4	0.15
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	4	0.15
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	4	0.15
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	4	0.15
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB2	2	0.15
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB3	2	0.15
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB2	2	0.15
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB3	2	0.15
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB2	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB3	2	0.15
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB2	9	0.15
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB3	9	0.15
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB2	9	0.15
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB3	9	0.15
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB2	9	0.15
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB3	9	0.15
(3,176)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	12	0.15
(3,176)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	12	0.15
(3,176)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	12	0.15
(3,176)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	12	0.15
(3,176)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	12	0.15
(3,176)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	12	0.15
(3,127)	1:705:A:VAL:H	1:702:A:LEU:HA	10	0.15
(3,108)	1:702:A:LEU:H	1:704:A:LEU:H	10	0.15
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	9	0.15
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	14	0.15
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	4	0.15
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	9	0.15
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	9	0.15
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	9	0.15
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	9	0.15
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	9	0.15
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	9	0.15
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	5	0.15
(3,46)	1:670:A:TRP:H	1:667:A:ALA:HA	6	0.15
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	14	0.15
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	14	0.15
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	14	0.15
(3,604)	1:693:A:ILE:HG21	1:690:A:GLY:HA2	7	0.14
(3,604)	1:693:A:ILE:HG21	1:690:A:GLY:HA3	7	0.14
(3,604)	1:693:A:ILE:HG22	1:690:A:GLY:HA2	7	0.14
(3,604)	1:693:A:ILE:HG22	1:690:A:GLY:HA3	7	0.14
(3,604)	1:693:A:ILE:HG23	1:690:A:GLY:HA2	7	0.14
(3,604)	1:693:A:ILE:HG23	1:690:A:GLY:HA3	7	0.14
(3,591)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.14
(3,591)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.14
(3,591)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.14
(3,585)	1:686:A:ILE:HD11	1:685:A:PHE:H	14	0.14
(3,585)	1:686:A:ILE:HD12	1:685:A:PHE:H	14	0.14
(3,585)	1:686:A:ILE:HD13	1:685:A:PHE:H	14	0.14
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	14	0.14
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	14	0.14
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	14	0.14
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	14	0.14
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	14	0.14
(3,543)	1:704:A:LEU:H	1:701:A:VAL:HA	6	0.14
(3,543)	1:704:A:LEU:H	1:701:A:VAL:HA	9	0.14
(3,515)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	14	0.14
(3,515)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	14	0.14
(3,515)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	14	0.14
(3,515)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	14	0.14
(3,515)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	14	0.14
(3,515)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	14	0.14
(3,508)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.14
(3,508)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.14
(3,508)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.14
(3,508)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.14
(3,508)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.14
(3,508)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.14
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	3	0.14
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	3	0.14
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	3	0.14
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	3	0.14
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	3	0.14
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	3	0.14
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	12	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	13	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	13	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	13	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	13	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	13	0.14
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	13	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	13	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	13	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	13	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	13	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	13	0.14
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	13	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	13	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	13	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	13	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	13	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	13	0.14
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	13	0.14
(3,458)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.14
(3,458)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.14
(3,441)	1:665:A:LYS:H	1:662:A:GLU:HA	13	0.14
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	1	0.14
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	1	0.14
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	1	0.14
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	1	0.14
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	1	0.14
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	1	0.14
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	3	0.14
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	3	0.14
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	3	0.14
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	3	0.14
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	3	0.14
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	3	0.14
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	8	0.14
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	8	0.14
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	8	0.14
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	8	0.14
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	8	0.14
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	8	0.14
(3,391)	1:693:A:ILE:HG21	1:690:A:GLY:HA2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,391)	1:693:A:ILE:HG21	1:690:A:GLY:HA3	7	0.14
(3,391)	1:693:A:ILE:HG22	1:690:A:GLY:HA2	7	0.14
(3,391)	1:693:A:ILE:HG22	1:690:A:GLY:HA3	7	0.14
(3,391)	1:693:A:ILE:HG23	1:690:A:GLY:HA2	7	0.14
(3,391)	1:693:A:ILE:HG23	1:690:A:GLY:HA3	7	0.14
(3,378)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.14
(3,378)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.14
(3,378)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.14
(3,372)	1:686:A:ILE:HD11	1:685:A:PHE:H	14	0.14
(3,372)	1:686:A:ILE:HD12	1:685:A:PHE:H	14	0.14
(3,372)	1:686:A:ILE:HD13	1:685:A:PHE:H	14	0.14
(3,295)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.14
(3,295)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.14
(3,295)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.14
(3,295)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.14
(3,295)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.14
(3,295)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	13	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	13	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	13	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	13	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	13	0.14
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	13	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	13	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	13	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	13	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	13	0.14
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	13	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	13	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	13	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	13	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	13	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	13	0.14
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	13	0.14
(3,245)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.14
(3,245)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.14
(3,228)	1:665:A:LYS:H	1:662:A:GLU:HA	13	0.14
(3,222)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	6	0.14
(3,222)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	6	0.14
(3,222)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	6	0.14
(3,222)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	6	0.14
(3,222)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	6	0.14
(3,222)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	6	0.14
(3,222)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	6	0.14
(3,222)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	6	0.14
(3,222)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	6	0.14
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	8	0.14
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	8	0.14
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	8	0.14
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	8	0.14
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	8	0.14
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	8	0.14
(3,178)	1:693:A:ILE:HG21	1:690:A:GLY:HA2	7	0.14
(3,178)	1:693:A:ILE:HG21	1:690:A:GLY:HA3	7	0.14
(3,178)	1:693:A:ILE:HG22	1:690:A:GLY:HA2	7	0.14
(3,178)	1:693:A:ILE:HG22	1:690:A:GLY:HA3	7	0.14
(3,178)	1:693:A:ILE:HG23	1:690:A:GLY:HA2	7	0.14
(3,178)	1:693:A:ILE:HG23	1:690:A:GLY:HA3	7	0.14
(3,177)	1:693:A:ILE:HD11	1:697:A:ILE:H	2	0.14
(3,177)	1:693:A:ILE:HD12	1:697:A:ILE:H	2	0.14
(3,177)	1:693:A:ILE:HD13	1:697:A:ILE:H	2	0.14
(3,165)	1:688:A:ILE:HG21	1:692:A:LEU:HG	2	0.14
(3,165)	1:688:A:ILE:HG22	1:692:A:LEU:HG	2	0.14
(3,165)	1:688:A:ILE:HG23	1:692:A:LEU:HG	2	0.14
(3,159)	1:686:A:ILE:HD11	1:685:A:PHE:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,159)	1:686:A:ILE:HD12	1:685:A:PHE:H	14	0.14
(3,159)	1:686:A:ILE:HD13	1:685:A:PHE:H	14	0.14
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	14	0.14
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	14	0.14
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	14	0.14
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	14	0.14
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	14	0.14
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	14	0.14
(3,132)	1:705:A:VAL:HG11	1:702:A:LEU:HA	14	0.14
(3,132)	1:705:A:VAL:HG12	1:702:A:LEU:HA	14	0.14
(3,132)	1:705:A:VAL:HG13	1:702:A:LEU:HA	14	0.14
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	11	0.14
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	13	0.14
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	8	0.14
(3,95)	1:685:A:PHE:H	1:684:A:ILE:H	13	0.14
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	14	0.14
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	14	0.14
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	14	0.14
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	14	0.14
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	14	0.14
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	14	0.14
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	1	0.14
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	1	0.14
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	1	0.14
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	4	0.14
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	4	0.14
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	4	0.14
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	4	0.14
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	4	0.14
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	4	0.14
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	12	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	5	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	10	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	10	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	10	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	10	0.14
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	10	0.14
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	7	0.14
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	7	0.14
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	7	0.14
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	7	0.14
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	7	0.14
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	7	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	5	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	5	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	5	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	5	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	5	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	5	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	5	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	5	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	13	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	13	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	13	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	13	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	13	0.14
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	13	0.14
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	13	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	13	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	13	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	13	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	13	0.14
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	13	0.14
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	9	0.14
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	14	0.14
(3,15)	1:665:A:LYS:H	1:662:A:GLU:HA	13	0.14
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	6	0.14
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	6	0.14
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	6	0.14
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	6	0.14
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	6	0.14
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	6	0.14
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	6	0.14
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	6	0.14
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	6	0.14
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	1	0.14
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	1	0.14
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	1	0.14
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	6	0.14
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	6	0.14
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	6	0.14
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	12	0.14
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	12	0.14
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	12	0.14
(3,617)	1:696:A:ARG:H	1:696:A:ARG:HE	2	0.13
(3,617)	1:696:A:ARG:H	1:696:A:ARG:HE	12	0.13
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	5	0.13
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	7	0.13
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD2	8	0.13
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD3	8	0.13
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	7	0.13
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	7	0.13
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	7	0.13
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	7	0.13
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	7	0.13
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	7	0.13
(3,562)	1:705:A:VAL:HG21	1:702:A:LEU:HG	4	0.13
(3,562)	1:705:A:VAL:HG22	1:702:A:LEU:HG	4	0.13
(3,562)	1:705:A:VAL:HG23	1:702:A:LEU:HG	4	0.13
(3,552)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	3	0.13
(3,552)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	3	0.13
(3,552)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	3	0.13
(3,552)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	3	0.13
(3,552)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,552)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	3	0.13
(3,552)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	3	0.13
(3,552)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	3	0.13
(3,552)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	3	0.13
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	5	0.13
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	7	0.13
(3,515)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	8	0.13
(3,515)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	8	0.13
(3,515)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	8	0.13
(3,515)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	8	0.13
(3,515)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	8	0.13
(3,515)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	8	0.13
(3,404)	1:696:A:ARG:H	1:696:A:ARG:HE	2	0.13
(3,404)	1:696:A:ARG:H	1:696:A:ARG:HE	12	0.13
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	13	0.13
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	13	0.13
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	13	0.13
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	13	0.13
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	13	0.13
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	13	0.13
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB2	3	0.13
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB3	3	0.13
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB2	3	0.13
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB3	3	0.13
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB2	3	0.13
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB3	3	0.13
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	5	0.13
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	7	0.13
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD2	8	0.13
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD3	8	0.13
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	13	0.13
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	13	0.13
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	13	0.13
(3,270)	1:672:A:TRP:HE1	1:671:A:ASN:H	6	0.13
(3,266)	1:671:A:ASN:H	1:672:A:TRP:HE1	6	0.13
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB2	4	0.13
(3,198)	1:698:A:VAL:HG11	1:702:A:LEU:HB3	4	0.13
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB2	4	0.13
(3,198)	1:698:A:VAL:HG12	1:702:A:LEU:HB3	4	0.13
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB2	4	0.13
(3,198)	1:698:A:VAL:HG13	1:702:A:LEU:HB3	4	0.13
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB2	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB3	3	0.13
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB2	3	0.13
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB3	3	0.13
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB2	3	0.13
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB3	3	0.13
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD2	8	0.13
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD3	8	0.13
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	7	0.13
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	7	0.13
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	7	0.13
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	7	0.13
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	7	0.13
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	7	0.13
(3,132)	1:705:A:VAL:HG11	1:702:A:LEU:HA	12	0.13
(3,132)	1:705:A:VAL:HG12	1:702:A:LEU:HA	12	0.13
(3,132)	1:705:A:VAL:HG13	1:702:A:LEU:HA	12	0.13
(3,126)	1:704:A:LEU:HD11	1:708:A:VAL:HG21	3	0.13
(3,126)	1:704:A:LEU:HD11	1:708:A:VAL:HG22	3	0.13
(3,126)	1:704:A:LEU:HD11	1:708:A:VAL:HG23	3	0.13
(3,126)	1:704:A:LEU:HD12	1:708:A:VAL:HG21	3	0.13
(3,126)	1:704:A:LEU:HD12	1:708:A:VAL:HG22	3	0.13
(3,126)	1:704:A:LEU:HD12	1:708:A:VAL:HG23	3	0.13
(3,126)	1:704:A:LEU:HD13	1:708:A:VAL:HG21	3	0.13
(3,126)	1:704:A:LEU:HD13	1:708:A:VAL:HG22	3	0.13
(3,126)	1:704:A:LEU:HD13	1:708:A:VAL:HG23	3	0.13
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	5	0.13
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	7	0.13
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	3	0.13
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	4	0.13
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	12	0.13
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE1	8	0.13
(3,89)	1:684:A:ILE:HD11	1:681:A:TYR:HE2	8	0.13
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE1	8	0.13
(3,89)	1:684:A:ILE:HD12	1:681:A:TYR:HE2	8	0.13
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE1	8	0.13
(3,89)	1:684:A:ILE:HD13	1:681:A:TYR:HE2	8	0.13
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	13	0.13
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	13	0.13
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	13	0.13
(3,57)	1:672:A:TRP:HE1	1:671:A:ASN:H	6	0.13
(3,53)	1:671:A:ASN:H	1:672:A:TRP:HE1	6	0.13
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	9	0.13
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	9	0.13
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	9	0.13
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	9	0.13
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	9	0.13
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	1	0.13
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	1	0.13
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	1	0.13
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	1	0.13
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	1	0.13
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	1	0.13
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	12	0.13
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	12	0.13
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	12	0.13
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	12	0.13
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	12	0.13
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	12	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	2	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	2	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	2	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	3	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	3	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	3	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	5	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	5	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	5	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	7	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	7	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	7	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	8	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	8	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	8	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	9	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	9	0.13
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	9	0.13
(1,3)	1:666:A:TRP:HE1	2:801:B:QOJ:H312	11	0.13
(3,622)	1:698:A:VAL:HG11	1:695:A:LEU:HG	6	0.12
(3,622)	1:698:A:VAL:HG12	1:695:A:LEU:HG	6	0.12
(3,622)	1:698:A:VAL:HG13	1:695:A:LEU:HG	6	0.12
(3,622)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.12
(3,622)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.12
(3,622)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,612)	1:695:A:LEU:HD21	1:698:A:VAL:HB	12	0.12
(3,612)	1:695:A:LEU:HD22	1:698:A:VAL:HB	12	0.12
(3,612)	1:695:A:LEU:HD23	1:698:A:VAL:HB	12	0.12
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD2	14	0.12
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD3	14	0.12
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	6	0.12
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	6	0.12
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	6	0.12
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	6	0.12
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	6	0.12
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	6	0.12
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	8	0.12
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	8	0.12
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	8	0.12
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	8	0.12
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	8	0.12
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	8	0.12
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	9	0.12
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	9	0.12
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	9	0.12
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	9	0.12
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	9	0.12
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	9	0.12
(3,562)	1:705:A:VAL:HG21	1:702:A:LEU:HG	8	0.12
(3,562)	1:705:A:VAL:HG22	1:702:A:LEU:HG	8	0.12
(3,562)	1:705:A:VAL:HG23	1:702:A:LEU:HG	8	0.12
(3,543)	1:704:A:LEU:H	1:701:A:VAL:HA	1	0.12
(3,499)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.12
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	11	0.12
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	11	0.12
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	11	0.12
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	11	0.12
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	11	0.12
(3,498)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	11	0.12
(3,492)	1:676:A:THR:HG21	1:679:A:LEU:H	8	0.12
(3,492)	1:676:A:THR:HG22	1:679:A:LEU:H	8	0.12
(3,492)	1:676:A:THR:HG23	1:679:A:LEU:H	8	0.12
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	14	0.12
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	14	0.12
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	14	0.12
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	14	0.12
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,461)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	14	0.12
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	14	0.12
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	14	0.12
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	14	0.12
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	14	0.12
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	14	0.12
(3,461)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	14	0.12
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	14	0.12
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	14	0.12
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	14	0.12
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	14	0.12
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	14	0.12
(3,461)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	14	0.12
(3,458)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.12
(3,455)	1:667:A:ALA:H	1:664:A:ASP:HA	5	0.12
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.12
(3,409)	1:698:A:VAL:HG11	1:695:A:LEU:HG	6	0.12
(3,409)	1:698:A:VAL:HG12	1:695:A:LEU:HG	6	0.12
(3,409)	1:698:A:VAL:HG13	1:695:A:LEU:HG	6	0.12
(3,409)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.12
(3,409)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.12
(3,409)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.12
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	4	0.12
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	4	0.12
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	4	0.12
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	4	0.12
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	4	0.12
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	4	0.12
(3,399)	1:695:A:LEU:HD21	1:698:A:VAL:HB	12	0.12
(3,399)	1:695:A:LEU:HD22	1:698:A:VAL:HB	12	0.12
(3,399)	1:695:A:LEU:HD23	1:698:A:VAL:HB	12	0.12
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB2	4	0.12
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB3	4	0.12
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB2	4	0.12
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB3	4	0.12
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB2	4	0.12
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB3	4	0.12
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB2	5	0.12
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB3	5	0.12
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB2	5	0.12
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB3	5	0.12
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB3	5	0.12
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	9	0.12
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	9	0.12
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	9	0.12
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	9	0.12
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	9	0.12
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	9	0.12
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD2	14	0.12
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD3	14	0.12
(3,350)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	8	0.12
(3,350)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	8	0.12
(3,350)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	8	0.12
(3,350)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	8	0.12
(3,350)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	8	0.12
(3,350)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	8	0.12
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	2	0.12
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	2	0.12
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	2	0.12
(3,346)	1:705:A:VAL:HG11	1:706:A:ASN:HA	8	0.12
(3,346)	1:705:A:VAL:HG12	1:706:A:ASN:HA	8	0.12
(3,346)	1:705:A:VAL:HG13	1:706:A:ASN:HA	8	0.12
(3,340)	1:705:A:VAL:H	1:702:A:LEU:HA	7	0.12
(3,340)	1:705:A:VAL:H	1:702:A:LEU:HA	14	0.12
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	7	0.12
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	7	0.12
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	7	0.12
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	7	0.12
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	7	0.12
(3,285)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	7	0.12
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	14	0.12
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	14	0.12
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	14	0.12
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	14	0.12
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	14	0.12
(3,248)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	14	0.12
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	14	0.12
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	14	0.12
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	14	0.12
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	14	0.12
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	14	0.12
(3,248)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	14	0.12
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	14	0.12
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	14	0.12
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	14	0.12
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	14	0.12
(3,248)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	14	0.12
(3,245)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.12
(3,242)	1:667:A:ALA:H	1:664:A:ASP:HA	5	0.12
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.12
(3,212)	1:701:A:VAL:HG11	1:698:A:VAL:HA	6	0.12
(3,212)	1:701:A:VAL:HG12	1:698:A:VAL:HA	6	0.12
(3,212)	1:701:A:VAL:HG13	1:698:A:VAL:HA	6	0.12
(3,196)	1:698:A:VAL:HG11	1:695:A:LEU:HG	6	0.12
(3,196)	1:698:A:VAL:HG12	1:695:A:LEU:HG	6	0.12
(3,196)	1:698:A:VAL:HG13	1:695:A:LEU:HG	6	0.12
(3,196)	1:698:A:VAL:HG11	1:695:A:LEU:HG	9	0.12
(3,196)	1:698:A:VAL:HG12	1:695:A:LEU:HG	9	0.12
(3,196)	1:698:A:VAL:HG13	1:695:A:LEU:HG	9	0.12
(3,186)	1:695:A:LEU:HD21	1:698:A:VAL:HB	12	0.12
(3,186)	1:695:A:LEU:HD22	1:698:A:VAL:HB	12	0.12
(3,186)	1:695:A:LEU:HD23	1:698:A:VAL:HB	12	0.12
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	13	0.12
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	13	0.12
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	13	0.12
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	13	0.12
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	13	0.12
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	13	0.12
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD2	14	0.12
(3,185)	1:695:A:LEU:HD21	1:696:A:ARG:HD3	14	0.12
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD2	14	0.12
(3,185)	1:695:A:LEU:HD22	1:696:A:ARG:HD3	14	0.12
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD2	14	0.12
(3,185)	1:695:A:LEU:HD23	1:696:A:ARG:HD3	14	0.12
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB2	4	0.12
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB3	4	0.12
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB2	4	0.12
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB3	4	0.12
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB2	4	0.12
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB3	4	0.12
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB2	5	0.12
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB3	5	0.12
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB2	5	0.12
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB3	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB2	5	0.12
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB3	5	0.12
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	9	0.12
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	9	0.12
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	9	0.12
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	9	0.12
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	9	0.12
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	9	0.12
(3,177)	1:693:A:ILE:HD11	1:697:A:ILE:H	6	0.12
(3,177)	1:693:A:ILE:HD12	1:697:A:ILE:H	6	0.12
(3,177)	1:693:A:ILE:HD13	1:697:A:ILE:H	6	0.12
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD2	14	0.12
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD3	14	0.12
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	6	0.12
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	6	0.12
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	6	0.12
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	6	0.12
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	6	0.12
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	6	0.12
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	9	0.12
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	9	0.12
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	9	0.12
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	9	0.12
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	9	0.12
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	9	0.12
(3,136)	1:705:A:VAL:HG21	1:702:A:LEU:HG	8	0.12
(3,136)	1:705:A:VAL:HG22	1:702:A:LEU:HG	8	0.12
(3,136)	1:705:A:VAL:HG23	1:702:A:LEU:HG	8	0.12
(3,132)	1:705:A:VAL:HG11	1:702:A:LEU:HA	5	0.12
(3,132)	1:705:A:VAL:HG12	1:702:A:LEU:HA	5	0.12
(3,132)	1:705:A:VAL:HG13	1:702:A:LEU:HA	5	0.12
(3,132)	1:705:A:VAL:HG11	1:702:A:LEU:HA	6	0.12
(3,132)	1:705:A:VAL:HG12	1:702:A:LEU:HA	6	0.12
(3,132)	1:705:A:VAL:HG13	1:702:A:LEU:HA	6	0.12
(3,132)	1:705:A:VAL:HG11	1:702:A:LEU:HA	7	0.12
(3,132)	1:705:A:VAL:HG12	1:702:A:LEU:HA	7	0.12
(3,132)	1:705:A:VAL:HG13	1:702:A:LEU:HA	7	0.12
(3,127)	1:705:A:VAL:H	1:702:A:LEU:HA	7	0.12
(3,127)	1:705:A:VAL:H	1:702:A:LEU:HA	14	0.12
(3,105)	1:702:A:LEU:H	1:700:A:ALA:H	2	0.12
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	1	0.12
(3,98)	1:686:A:ILE:H	1:687:A:ILE:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	2	0.12
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	13	0.12
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	4	0.12
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	4	0.12
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	4	0.12
(3,73)	1:678:A:TRP:HE1	1:682:A:ILE:H	10	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD11	9	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD12	9	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD13	9	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD21	9	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD22	9	0.12
(3,72)	1:678:A:TRP:HE1	1:679:A:LEU:HD23	9	0.12
(3,66)	1:676:A:THR:HG21	1:679:A:LEU:H	8	0.12
(3,66)	1:676:A:THR:HG22	1:679:A:LEU:H	8	0.12
(3,66)	1:676:A:THR:HG23	1:679:A:LEU:H	8	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD11	14	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD12	14	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD13	14	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD21	14	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD22	14	0.12
(3,35)	1:667:A:ALA:HB1	1:663:A:LEU:HD23	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD11	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD12	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD13	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD21	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD22	14	0.12
(3,35)	1:667:A:ALA:HB2	1:663:A:LEU:HD23	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD11	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD12	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD13	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD21	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD22	14	0.12
(3,35)	1:667:A:ALA:HB3	1:663:A:LEU:HD23	14	0.12
(3,32)	1:667:A:ALA:H	1:666:A:TRP:HD1	11	0.12
(3,29)	1:667:A:ALA:H	1:664:A:ASP:HA	5	0.12
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	13	0.12
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	4	0.12
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	4	0.12
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	4	0.12
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	11	0.12
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	11	0.12
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,622)	1:698:A:VAL:HG11	1:695:A:LEU:HG	8	0.11
(3,622)	1:698:A:VAL:HG12	1:695:A:LEU:HG	8	0.11
(3,622)	1:698:A:VAL:HG13	1:695:A:LEU:HG	8	0.11
(3,606)	1:693:A:ILE:HG21	1:694:A:GLY:H	1	0.11
(3,606)	1:693:A:ILE:HG22	1:694:A:GLY:H	1	0.11
(3,606)	1:693:A:ILE:HG23	1:694:A:GLY:H	1	0.11
(3,599)	1:692:A:LEU:HD11	1:691:A:SER:HB2	10	0.11
(3,599)	1:692:A:LEU:HD11	1:691:A:SER:HB3	10	0.11
(3,599)	1:692:A:LEU:HD12	1:691:A:SER:HB2	10	0.11
(3,599)	1:692:A:LEU:HD12	1:691:A:SER:HB3	10	0.11
(3,599)	1:692:A:LEU:HD13	1:691:A:SER:HB2	10	0.11
(3,599)	1:692:A:LEU:HD13	1:691:A:SER:HB3	10	0.11
(3,595)	1:690:A:GLY:H	1:689:A:VAL:H	11	0.11
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE1	9	0.11
(3,594)	1:689:A:VAL:HG21	1:685:A:PHE:HE2	9	0.11
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE1	9	0.11
(3,594)	1:689:A:VAL:HG22	1:685:A:PHE:HE2	9	0.11
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE1	9	0.11
(3,594)	1:689:A:VAL:HG23	1:685:A:PHE:HE2	9	0.11
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD2	2	0.11
(3,577)	1:707:A:ARG:H	1:707:A:ARG:HD3	2	0.11
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	2	0.11
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	2	0.11
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	2	0.11
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	2	0.11
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	2	0.11
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	2	0.11
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.11
(3,563)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.11
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.11
(3,563)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.11
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.11
(3,563)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.11
(3,529)	1:689:A:VAL:H	1:690:A:GLY:H	11	0.11
(3,514)	1:684:A:ILE:HD11	1:681:A:TYR:HA	13	0.11
(3,514)	1:684:A:ILE:HD12	1:681:A:TYR:HA	13	0.11
(3,514)	1:684:A:ILE:HD13	1:681:A:TYR:HA	13	0.11
(3,508)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.11
(3,508)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.11
(3,508)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.11
(3,508)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.11
(3,508)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,508)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.11
(3,505)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11
(3,505)	1:681:A:TYR:H	1:682:A:ILE:H	14	0.11
(3,490)	1:676:A:THR:HG21	1:669:A:LEU:HA	13	0.11
(3,490)	1:676:A:THR:HG22	1:669:A:LEU:HA	13	0.11
(3,490)	1:676:A:THR:HG23	1:669:A:LEU:HA	13	0.11
(3,485)	1:674:A:ASP:H	1:677:A:ASN:H	8	0.11
(3,480)	1:672:A:TRP:H	1:671:A:ASN:H	8	0.11
(3,476)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	1	0.11
(3,476)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	1	0.11
(3,476)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	1	0.11
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.11
(3,437)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.11
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	11	0.11
(3,427)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	11	0.11
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	11	0.11
(3,427)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	11	0.11
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	11	0.11
(3,427)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	11	0.11
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	11	0.11
(3,427)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	11	0.11
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	11	0.11
(3,427)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	11	0.11
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	11	0.11
(3,427)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	11	0.11
(3,409)	1:698:A:VAL:HG11	1:695:A:LEU:HG	8	0.11
(3,409)	1:698:A:VAL:HG12	1:695:A:LEU:HG	8	0.11
(3,409)	1:698:A:VAL:HG13	1:695:A:LEU:HG	8	0.11
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE1	12	0.11
(3,401)	1:695:A:LEU:HD21	1:699:A:PHE:HE2	12	0.11
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE1	12	0.11
(3,401)	1:695:A:LEU:HD22	1:699:A:PHE:HE2	12	0.11
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE1	12	0.11
(3,401)	1:695:A:LEU:HD23	1:699:A:PHE:HE2	12	0.11
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB2	8	0.11
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB3	8	0.11
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB2	8	0.11
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB3	8	0.11
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB2	8	0.11
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB3	8	0.11
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB2	13	0.11
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB3	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB2	13	0.11
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB3	13	0.11
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB2	13	0.11
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB3	13	0.11
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	4	0.11
(3,394)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	4	0.11
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	4	0.11
(3,394)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	4	0.11
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	4	0.11
(3,394)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	4	0.11
(3,393)	1:693:A:ILE:HG21	1:694:A:GLY:H	1	0.11
(3,393)	1:693:A:ILE:HG22	1:694:A:GLY:H	1	0.11
(3,393)	1:693:A:ILE:HG23	1:694:A:GLY:H	1	0.11
(3,386)	1:692:A:LEU:HD11	1:691:A:SER:HB2	10	0.11
(3,386)	1:692:A:LEU:HD11	1:691:A:SER:HB3	10	0.11
(3,386)	1:692:A:LEU:HD12	1:691:A:SER:HB2	10	0.11
(3,386)	1:692:A:LEU:HD12	1:691:A:SER:HB3	10	0.11
(3,386)	1:692:A:LEU:HD13	1:691:A:SER:HB2	10	0.11
(3,386)	1:692:A:LEU:HD13	1:691:A:SER:HB3	10	0.11
(3,382)	1:690:A:GLY:H	1:689:A:VAL:H	11	0.11
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD2	2	0.11
(3,364)	1:707:A:ARG:H	1:707:A:ARG:HD3	2	0.11
(3,348)	1:705:A:VAL:HG21	1:701:A:VAL:HA	4	0.11
(3,348)	1:705:A:VAL:HG22	1:701:A:VAL:HA	4	0.11
(3,348)	1:705:A:VAL:HG23	1:701:A:VAL:HA	4	0.11
(3,301)	1:684:A:ILE:HD11	1:681:A:TYR:HA	13	0.11
(3,301)	1:684:A:ILE:HD12	1:681:A:TYR:HA	13	0.11
(3,301)	1:684:A:ILE:HD13	1:681:A:TYR:HA	13	0.11
(3,295)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.11
(3,295)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.11
(3,295)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.11
(3,295)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.11
(3,295)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.11
(3,295)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.11
(3,292)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11
(3,292)	1:681:A:TYR:H	1:682:A:ILE:H	14	0.11
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	7	0.11
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	7	0.11
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	7	0.11
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	8	0.11
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	8	0.11
(3,284)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,277)	1:676:A:THR:HG21	1:669:A:LEU:HA	13	0.11
(3,277)	1:676:A:THR:HG22	1:669:A:LEU:HA	13	0.11
(3,277)	1:676:A:THR:HG23	1:669:A:LEU:HA	13	0.11
(3,272)	1:674:A:ASP:H	1:677:A:ASN:H	8	0.11
(3,270)	1:672:A:TRP:HE1	1:671:A:ASN:H	13	0.11
(3,266)	1:671:A:ASN:H	1:672:A:TRP:HE1	13	0.11
(3,263)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	1	0.11
(3,263)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	1	0.11
(3,263)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	1	0.11
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.11
(3,224)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.11
(3,196)	1:698:A:VAL:HG11	1:695:A:LEU:HG	8	0.11
(3,196)	1:698:A:VAL:HG12	1:695:A:LEU:HG	8	0.11
(3,196)	1:698:A:VAL:HG13	1:695:A:LEU:HG	8	0.11
(3,194)	1:697:A:ILE:HG21	1:700:A:ALA:HB1	13	0.11
(3,194)	1:697:A:ILE:HG21	1:700:A:ALA:HB2	13	0.11
(3,194)	1:697:A:ILE:HG21	1:700:A:ALA:HB3	13	0.11
(3,194)	1:697:A:ILE:HG22	1:700:A:ALA:HB1	13	0.11
(3,194)	1:697:A:ILE:HG22	1:700:A:ALA:HB2	13	0.11
(3,194)	1:697:A:ILE:HG22	1:700:A:ALA:HB3	13	0.11
(3,194)	1:697:A:ILE:HG23	1:700:A:ALA:HB1	13	0.11
(3,194)	1:697:A:ILE:HG23	1:700:A:ALA:HB2	13	0.11
(3,194)	1:697:A:ILE:HG23	1:700:A:ALA:HB3	13	0.11
(3,192)	1:697:A:ILE:HG21	1:694:A:GLY:HA2	8	0.11
(3,192)	1:697:A:ILE:HG21	1:694:A:GLY:HA3	8	0.11
(3,192)	1:697:A:ILE:HG22	1:694:A:GLY:HA2	8	0.11
(3,192)	1:697:A:ILE:HG22	1:694:A:GLY:HA3	8	0.11
(3,192)	1:697:A:ILE:HG23	1:694:A:GLY:HA2	8	0.11
(3,192)	1:697:A:ILE:HG23	1:694:A:GLY:HA3	8	0.11
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB2	8	0.11
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB3	8	0.11
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB2	8	0.11
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB3	8	0.11
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB2	8	0.11
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB3	8	0.11
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB2	13	0.11
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB3	13	0.11
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB2	13	0.11
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB3	13	0.11
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB2	13	0.11
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB3	13	0.11
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,181)	1:693:A:ILE:HG21	1:696:A:ARG:HG3	4	0.11
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG2	4	0.11
(3,181)	1:693:A:ILE:HG22	1:696:A:ARG:HG3	4	0.11
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG2	4	0.11
(3,181)	1:693:A:ILE:HG23	1:696:A:ARG:HG3	4	0.11
(3,180)	1:693:A:ILE:HG21	1:694:A:GLY:H	1	0.11
(3,180)	1:693:A:ILE:HG22	1:694:A:GLY:H	1	0.11
(3,180)	1:693:A:ILE:HG23	1:694:A:GLY:H	1	0.11
(3,175)	1:692:A:LEU:HD21	1:696:A:ARG:HH11	14	0.11
(3,173)	1:692:A:LEU:HD11	1:691:A:SER:HB2	10	0.11
(3,173)	1:692:A:LEU:HD11	1:691:A:SER:HB3	10	0.11
(3,173)	1:692:A:LEU:HD12	1:691:A:SER:HB2	10	0.11
(3,173)	1:692:A:LEU:HD12	1:691:A:SER:HB3	10	0.11
(3,173)	1:692:A:LEU:HD13	1:691:A:SER:HB2	10	0.11
(3,173)	1:692:A:LEU:HD13	1:691:A:SER:HB3	10	0.11
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD2	2	0.11
(3,151)	1:707:A:ARG:H	1:707:A:ARG:HD3	2	0.11
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	2	0.11
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	2	0.11
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	2	0.11
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	2	0.11
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	2	0.11
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	2	0.11
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB2	13	0.11
(3,137)	1:705:A:VAL:HG21	1:706:A:ASN:HB3	13	0.11
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB2	13	0.11
(3,137)	1:705:A:VAL:HG22	1:706:A:ASN:HB3	13	0.11
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB2	13	0.11
(3,137)	1:705:A:VAL:HG23	1:706:A:ASN:HB3	13	0.11
(3,135)	1:705:A:VAL:HG21	1:701:A:VAL:HA	4	0.11
(3,135)	1:705:A:VAL:HG22	1:701:A:VAL:HA	4	0.11
(3,135)	1:705:A:VAL:HG23	1:701:A:VAL:HA	4	0.11
(3,132)	1:705:A:VAL:HG11	1:702:A:LEU:HA	2	0.11
(3,132)	1:705:A:VAL:HG12	1:702:A:LEU:HA	2	0.11
(3,132)	1:705:A:VAL:HG13	1:702:A:LEU:HA	2	0.11
(3,103)	1:689:A:VAL:H	1:690:A:GLY:H	11	0.11
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	11	0.11
(3,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	13	0.11
(3,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	13	0.11
(3,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	13	0.11
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	11	0.11
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	11	0.11
(3,83)	1:682:A:ILE:HD11	1:681:A:TYR:H	14	0.11
(3,83)	1:682:A:ILE:HD12	1:681:A:TYR:H	14	0.11
(3,83)	1:682:A:ILE:HD13	1:681:A:TYR:H	14	0.11
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD1	11	0.11
(3,82)	1:682:A:ILE:HG21	1:685:A:PHE:HD2	11	0.11
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD1	11	0.11
(3,82)	1:682:A:ILE:HG22	1:685:A:PHE:HD2	11	0.11
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD1	11	0.11
(3,82)	1:682:A:ILE:HG23	1:685:A:PHE:HD2	11	0.11
(3,79)	1:681:A:TYR:H	1:682:A:ILE:H	3	0.11
(3,79)	1:681:A:TYR:H	1:682:A:ILE:H	14	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	7	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	7	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	7	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD11	8	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD12	8	0.11
(3,71)	1:678:A:TRP:HE1	1:675:A:ILE:HD13	8	0.11
(3,64)	1:676:A:THR:HG21	1:669:A:LEU:HA	13	0.11
(3,64)	1:676:A:THR:HG22	1:669:A:LEU:HA	13	0.11
(3,64)	1:676:A:THR:HG23	1:669:A:LEU:HA	13	0.11
(3,59)	1:674:A:ASP:H	1:677:A:ASN:H	8	0.11
(3,57)	1:672:A:TRP:HE1	1:671:A:ASN:H	13	0.11
(3,54)	1:672:A:TRP:H	1:671:A:ASN:H	8	0.11
(3,53)	1:671:A:ASN:H	1:672:A:TRP:HE1	13	0.11
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	1	0.11
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	1	0.11
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	1	0.11
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	1	0.11
(3,11)	1:664:A:ASP:H	1:663:A:LEU:HA	12	0.11
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	0.11
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	0.11
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	0.11
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	0.11
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG12	6	0.11
(2,16)	1:693:A:ILE:H	1:693:A:ILE:HG13	6	0.11
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	10	0.11
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	10	0.11
(2,4)	1:666:A:TRP:HE1	1:666:A:TRP:HZ2	10	0.11
(3,518)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	7	0.1
(3,518)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	7	0.1
(3,518)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,518)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	7	0.1
(3,518)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	7	0.1
(3,518)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	7	0.1
(3,514)	1:684:A:ILE:HD11	1:681:A:TYR:HA	11	0.1
(3,514)	1:684:A:ILE:HD12	1:681:A:TYR:HA	11	0.1
(3,514)	1:684:A:ILE:HD13	1:681:A:TYR:HA	11	0.1
(3,505)	1:681:A:TYR:H	1:682:A:ILE:H	11	0.1
(3,476)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	7	0.1
(3,476)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	7	0.1
(3,476)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	7	0.1
(3,466)	1:669:A:LEU:H	1:666:A:TRP:HA	4	0.1
(3,402)	1:696:A:ARG:H	1:693:A:ILE:HA	12	0.1
(3,399)	1:695:A:LEU:HD21	1:698:A:VAL:HB	2	0.1
(3,399)	1:695:A:LEU:HD22	1:698:A:VAL:HB	2	0.1
(3,399)	1:695:A:LEU:HD23	1:698:A:VAL:HB	2	0.1
(3,399)	1:695:A:LEU:HD21	1:698:A:VAL:HB	14	0.1
(3,399)	1:695:A:LEU:HD22	1:698:A:VAL:HB	14	0.1
(3,399)	1:695:A:LEU:HD23	1:698:A:VAL:HB	14	0.1
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB2	1	0.1
(3,397)	1:695:A:LEU:HD11	1:691:A:SER:HB3	1	0.1
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB2	1	0.1
(3,397)	1:695:A:LEU:HD12	1:691:A:SER:HB3	1	0.1
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB2	1	0.1
(3,397)	1:695:A:LEU:HD13	1:691:A:SER:HB3	1	0.1
(3,301)	1:684:A:ILE:HD11	1:681:A:TYR:HA	11	0.1
(3,301)	1:684:A:ILE:HD12	1:681:A:TYR:HA	11	0.1
(3,301)	1:684:A:ILE:HD13	1:681:A:TYR:HA	11	0.1
(3,292)	1:681:A:TYR:H	1:682:A:ILE:H	11	0.1
(3,263)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	7	0.1
(3,263)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	7	0.1
(3,263)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	7	0.1
(3,253)	1:669:A:LEU:H	1:666:A:TRP:HA	4	0.1
(3,222)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	10	0.1
(3,222)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	10	0.1
(3,222)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	10	0.1
(3,222)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	10	0.1
(3,222)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	10	0.1
(3,222)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	10	0.1
(3,222)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	10	0.1
(3,222)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	10	0.1
(3,222)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	10	0.1
(3,213)	1:701:A:VAL:HG21	1:698:A:VAL:HA	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,213)	1:701:A:VAL:HG22	1:698:A:VAL:HA	8	0.1
(3,213)	1:701:A:VAL:HG23	1:698:A:VAL:HA	8	0.1
(3,189)	1:696:A:ARG:H	1:693:A:ILE:HA	12	0.1
(3,186)	1:695:A:LEU:HD21	1:698:A:VAL:HB	2	0.1
(3,186)	1:695:A:LEU:HD22	1:698:A:VAL:HB	2	0.1
(3,186)	1:695:A:LEU:HD23	1:698:A:VAL:HB	2	0.1
(3,186)	1:695:A:LEU:HD21	1:698:A:VAL:HB	14	0.1
(3,186)	1:695:A:LEU:HD22	1:698:A:VAL:HB	14	0.1
(3,186)	1:695:A:LEU:HD23	1:698:A:VAL:HB	14	0.1
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB2	1	0.1
(3,184)	1:695:A:LEU:HD11	1:691:A:SER:HB3	1	0.1
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB2	1	0.1
(3,184)	1:695:A:LEU:HD12	1:691:A:SER:HB3	1	0.1
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB2	1	0.1
(3,184)	1:695:A:LEU:HD13	1:691:A:SER:HB3	1	0.1
(3,176)	1:693:A:ILE:HD11	1:694:A:GLY:HA2	6	0.1
(3,176)	1:693:A:ILE:HD11	1:694:A:GLY:HA3	6	0.1
(3,176)	1:693:A:ILE:HD12	1:694:A:GLY:HA2	6	0.1
(3,176)	1:693:A:ILE:HD12	1:694:A:GLY:HA3	6	0.1
(3,176)	1:693:A:ILE:HD13	1:694:A:GLY:HA2	6	0.1
(3,176)	1:693:A:ILE:HD13	1:694:A:GLY:HA3	6	0.1
(3,96)	1:685:A:PHE:H	1:686:A:ILE:H	1	0.1
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD1	7	0.1
(3,92)	1:684:A:ILE:HG21	1:685:A:PHE:HD2	7	0.1
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD1	7	0.1
(3,92)	1:684:A:ILE:HG22	1:685:A:PHE:HD2	7	0.1
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD1	7	0.1
(3,92)	1:684:A:ILE:HG23	1:685:A:PHE:HD2	7	0.1
(3,88)	1:684:A:ILE:HD11	1:681:A:TYR:HA	11	0.1
(3,88)	1:684:A:ILE:HD12	1:681:A:TYR:HA	11	0.1
(3,88)	1:684:A:ILE:HD13	1:681:A:TYR:HA	11	0.1
(3,79)	1:681:A:TYR:H	1:682:A:ILE:H	11	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	1	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD11	7	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD12	7	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD13	7	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD21	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD22	7	0.1
(3,56)	1:672:A:TRP:HE1	1:669:A:LEU:HD23	7	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD11	8	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD12	8	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD13	8	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD21	8	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD22	8	0.1
(3,51)	1:670:A:TRP:HE1	1:669:A:LEU:HD23	8	0.1
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB1	7	0.1
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB2	7	0.1
(3,50)	1:670:A:TRP:HE1	1:667:A:ALA:HB3	7	0.1
(3,45)	1:669:A:LEU:HD11	1:672:A:TRP:HZ3	4	0.1
(3,45)	1:669:A:LEU:HD12	1:672:A:TRP:HZ3	4	0.1
(3,45)	1:669:A:LEU:HD13	1:672:A:TRP:HZ3	4	0.1
(3,45)	1:669:A:LEU:HD21	1:672:A:TRP:HZ3	4	0.1
(3,45)	1:669:A:LEU:HD22	1:672:A:TRP:HZ3	4	0.1
(3,45)	1:669:A:LEU:HD23	1:672:A:TRP:HZ3	4	0.1
(3,40)	1:669:A:LEU:H	1:666:A:TRP:HA	4	0.1
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB1	10	0.1
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB2	10	0.1
(3,9)	1:663:A:LEU:HD21	1:667:A:ALA:HB3	10	0.1
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB1	10	0.1
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB2	10	0.1
(3,9)	1:663:A:LEU:HD22	1:667:A:ALA:HB3	10	0.1
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB1	10	0.1
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB2	10	0.1
(3,9)	1:663:A:LEU:HD23	1:667:A:ALA:HB3	10	0.1
(3,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD11	1:662:A:GLU:HG3	8	0.1
(3,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD12	1:662:A:GLU:HG3	8	0.1
(3,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD13	1:662:A:GLU:HG3	8	0.1
(3,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD21	1:662:A:GLU:HG3	8	0.1
(3,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD22	1:662:A:GLU:HG3	8	0.1
(3,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG2	8	0.1
(3,1)	1:661:A:LEU:HD23	1:662:A:GLU:HG3	8	0.1

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

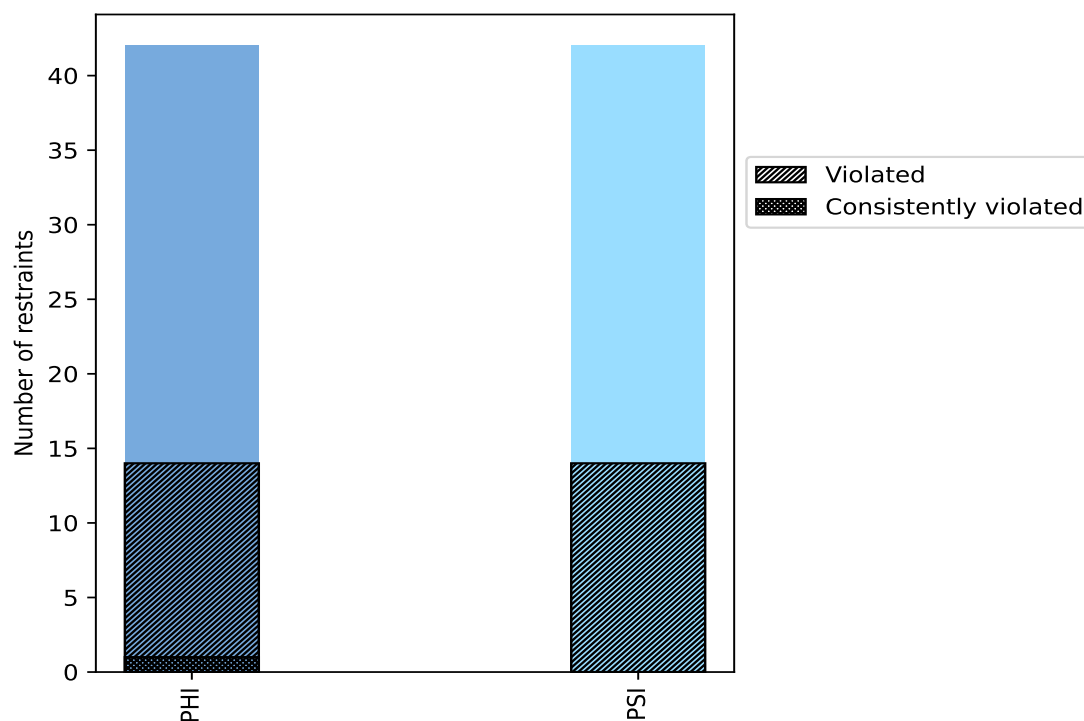
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	42	50.0	14	33.3	16.7	1	2.4	1.2
PSI	42	50.0	14	33.3	16.7	0	0.0	0.0
Total	84	100.0	28	33.3	33.3	1	1.2	1.2

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

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



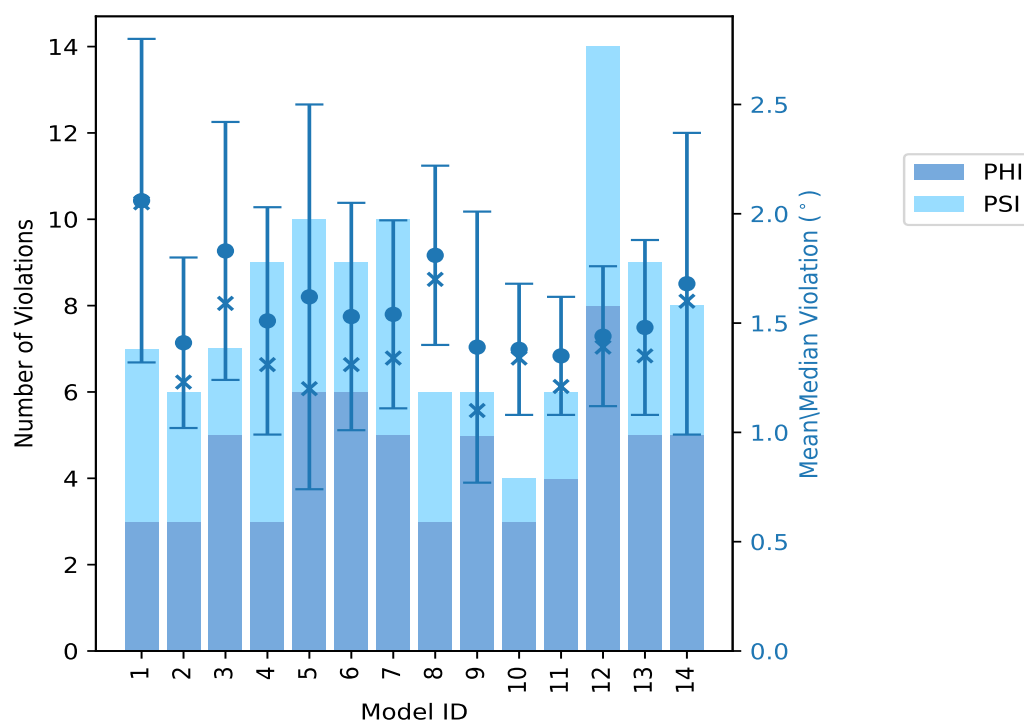
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	3	4	7	2.06	3.36	0.74	2.05
2	3	3	6	1.41	2.19	0.39	1.23
3	5	2	7	1.83	3.11	0.59	1.59
4	3	6	9	1.51	2.73	0.52	1.31
5	6	4	10	1.62	4.01	0.88	1.2
6	6	3	9	1.53	2.83	0.52	1.31
7	5	5	10	1.54	2.42	0.43	1.34
8	3	3	6	1.81	2.53	0.41	1.7
9	5	1	6	1.39	2.76	0.62	1.1
10	3	1	4	1.38	1.77	0.3	1.34
11	4	2	6	1.35	1.82	0.27	1.21
12	8	6	14	1.44	2.12	0.32	1.39
13	5	4	9	1.48	2.15	0.4	1.35
14	5	3	8	1.68	3.34	0.69	1.6

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

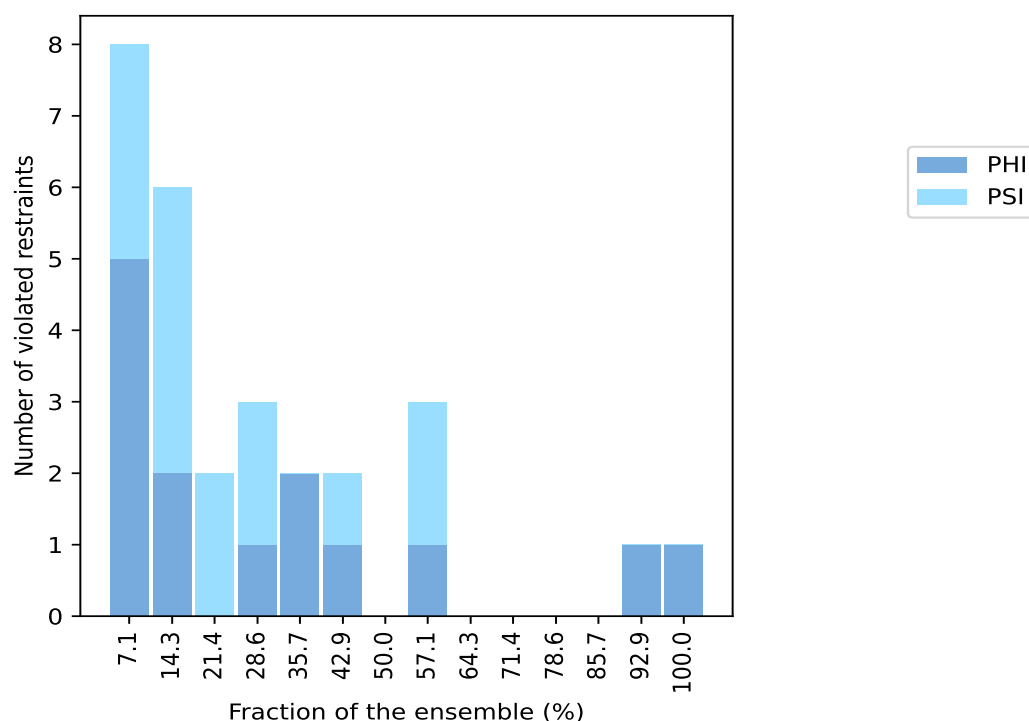
10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
5	3	8	1	7.1
2	4	6	2	14.3
0	2	2	3	21.4
1	2	3	4	28.6
2	0	2	5	35.7
1	1	2	6	42.9
0	0	0	7	50.0
1	2	3	8	57.1
0	0	0	9	64.3
0	0	0	10	71.4
0	0	0	11	78.6
0	0	0	12	85.7
1	0	1	13	92.9
1	0	1	14	100.0

¹ Number of models with violations

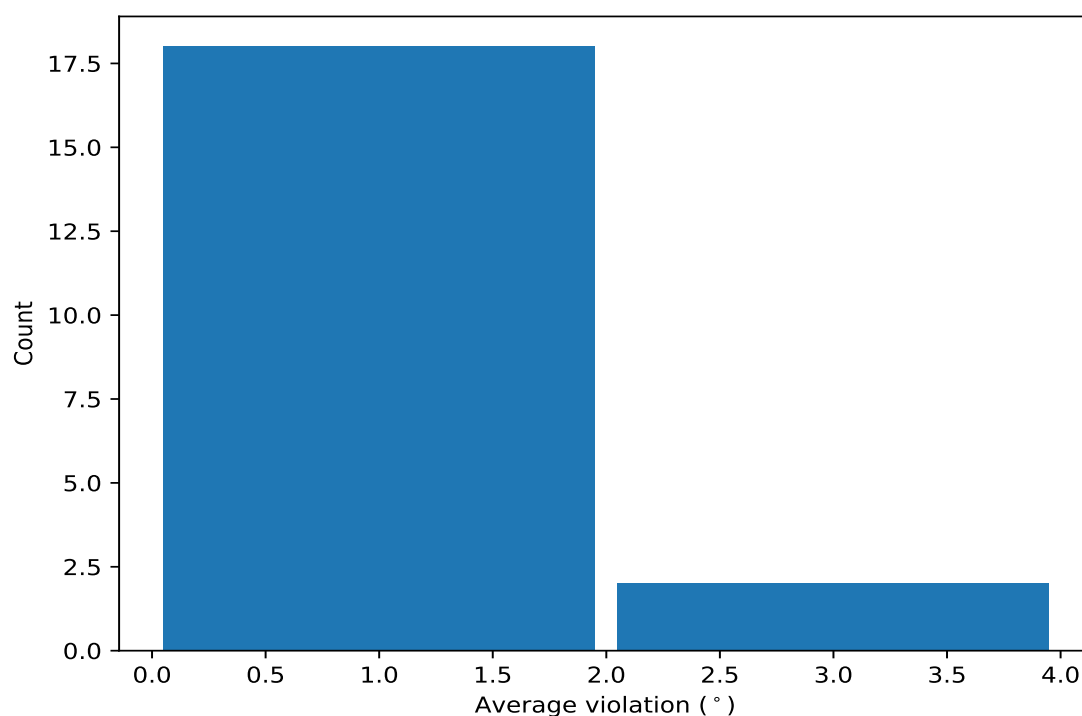
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

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

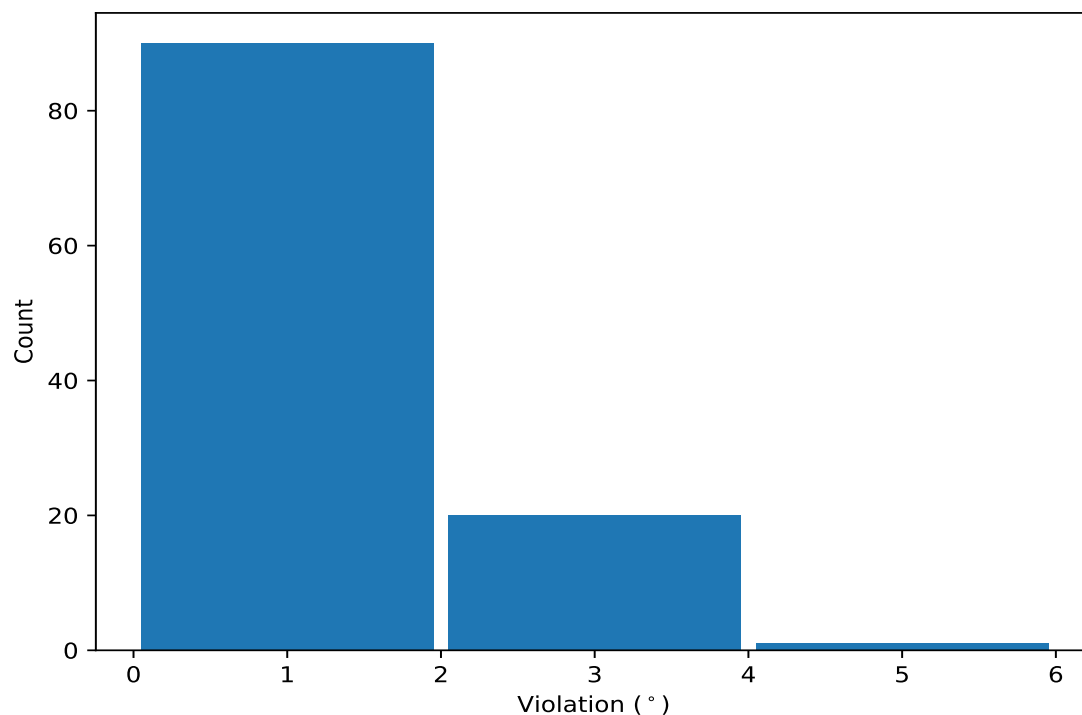
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	14	2.21	0.78	2.07
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	13	1.51	0.35	1.44
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	8	2.25	0.72	2.0
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	8	1.84	0.54	1.89
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	8	1.76	0.32	1.76
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	6	1.45	0.3	1.44
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	6	1.27	0.17	1.23
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	5	1.23	0.02	1.24
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	5	1.18	0.13	1.16
(1,20)	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	1:673:C:PHE:N	4	1.5	0.17	1.44
(1,63)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	4	1.39	0.42	1.18
(1,52)	1:692:C:LEU:N	1:692:C:LEU:CA	1:692:C:LEU:C	1:693:C:ILE:N	4	1.2	0.1	1.19
(1,58)	1:695:C:LEU:N	1:695:C:LEU:CA	1:695:C:LEU:C	1:696:C:ARG:N	3	1.33	0.16	1.31
(1,68)	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	1:701:C:VAL:N	3	1.08	0.07	1.07
(1,38)	1:684:C:ILE:N	1:684:C:ILE:CA	1:684:C:ILE:C	1:685:C:PHE:N	2	1.36	0.17	1.36
(1,65)	1:698:C:VAL:C	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	2	1.18	0.02	1.18
(1,64)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	2	1.14	0.08	1.14
(1,41)	1:685:C:PHE:C	1:686:C:ILE:N	1:686:C:ILE:CA	1:686:C:ILE:C	2	1.14	0.03	1.14
(1,40)	1:685:C:PHE:N	1:685:C:PHE:CA	1:685:C:PHE:C	1:686:C:ILE:N	2	1.14	0.09	1.14
(1,46)	1:688:C:ILE:N	1:688:C:ILE:CA	1:688:C:ILE:C	1:689:C:VAL:N	2	1.11	0.0	1.11

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

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

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

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	5	4.01
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1	3.36
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	14	3.34
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	3	3.11
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	6	2.83
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	9	2.76
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	4	2.73
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	1	2.6
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	8	2.53
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	7	2.42
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	1	2.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	5	2.32
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	2	2.19
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	13	2.15
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	8	2.14
(1,34)	1:682:C:ILE:N	1:682:C:ILE:CA	1:682:C:ILE:C	1:683:C:ARG:N	12	2.12
(1,63)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	3	2.1
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	1	2.05
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	12	2.01
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	13	2.0
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	4	2.0
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	7	1.97
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	13	1.89
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	3	1.88
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	6	1.88
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	7	1.88
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	7	1.82
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	11	1.82
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	14	1.81
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	10	1.77
(1,20)	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	1:673:C:PHE:N	8	1.77
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	5	1.76
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	14	1.76
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	1	1.75
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	6	1.73
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	8	1.64
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	14	1.64
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	12	1.63
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	12	1.63
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	11	1.6
(1,39)	1:684:C:ILE:C	1:685:C:PHE:N	1:685:C:PHE:CA	1:685:C:PHE:C	3	1.59
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	2	1.58
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	14	1.57
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	10	1.55
(1,58)	1:695:C:LEU:N	1:695:C:LEU:CA	1:695:C:LEU:C	1:696:C:ARG:N	12	1.54
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	12	1.54
(1,38)	1:684:C:ILE:N	1:684:C:ILE:CA	1:684:C:ILE:C	1:685:C:PHE:N	3	1.53
(1,35)	1:682:C:ILE:C	1:683:C:ARG:N	1:683:C:ARG:CA	1:683:C:ARG:C	12	1.53
(1,20)	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	1:673:C:PHE:N	4	1.53
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	4	1.52
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	8	1.44
(1,29)	1:677:C:ASN:C	1:678:C:TRP:N	1:678:C:TRP:CA	1:678:C:TRP:C	13	1.43
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	3	1.42
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	9	1.37
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	6	1.35
(1,20)	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	1:673:C:PHE:N	7	1.35
(1,20)	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	1:673:C:PHE:N	13	1.35
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	8	1.33
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	7	1.33
(1,52)	1:692:C:LEU:N	1:692:C:LEU:CA	1:692:C:LEU:C	1:693:C:ILE:N	2	1.32
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	4	1.31
(1,58)	1:695:C:LEU:N	1:695:C:LEU:CA	1:695:C:LEU:C	1:696:C:ARG:N	6	1.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,63)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	6	1.28
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	5	1.26
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	12	1.25
(1,52)	1:692:C:LEU:N	1:692:C:LEU:CA	1:692:C:LEU:C	1:693:C:ILE:N	4	1.25
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	12	1.24
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	14	1.24
(1,64)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	11	1.23
(1,40)	1:685:C:PHE:N	1:685:C:PHE:CA	1:685:C:PHE:C	1:686:C:ILE:N	7	1.23
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	5	1.22
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	7	1.22
(1,44)	1:687:C:ILE:N	1:687:C:ILE:CA	1:687:C:ILE:C	1:688:C:ILE:N	6	1.21
(1,65)	1:698:C:VAL:C	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	12	1.2
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	11	1.2
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	3	1.19
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	5	1.19
(1,38)	1:684:C:ILE:N	1:684:C:ILE:CA	1:684:C:ILE:C	1:685:C:PHE:N	5	1.19
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	13	1.19
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	13	1.18
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	12	1.18
(1,68)	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	1:701:C:VAL:N	1	1.17
(1,41)	1:685:C:PHE:C	1:686:C:ILE:N	1:686:C:ILE:CA	1:686:C:ILE:C	12	1.17
(1,65)	1:698:C:VAL:C	1:699:C:PHE:N	1:699:C:PHE:CA	1:699:C:PHE:C	11	1.16
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	6	1.16
(1,58)	1:695:C:LEU:N	1:695:C:LEU:CA	1:695:C:LEU:C	1:696:C:ARG:N	2	1.15
(1,52)	1:692:C:LEU:N	1:692:C:LEU:CA	1:692:C:LEU:C	1:693:C:ILE:N	10	1.14
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	9	1.12
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	13	1.12
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	2	1.11
(1,46)	1:688:C:ILE:N	1:688:C:ILE:CA	1:688:C:ILE:C	1:689:C:VAL:N	1	1.11
(1,46)	1:688:C:ILE:N	1:688:C:ILE:CA	1:688:C:ILE:C	1:689:C:VAL:N	2	1.11
(1,41)	1:685:C:PHE:C	1:686:C:ILE:N	1:686:C:ILE:CA	1:686:C:ILE:C	7	1.11
(1,63)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	5	1.09
(1,63)	1:697:C:ILE:C	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	14	1.08
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	5	1.08
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	4	1.08
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	5	1.08
(1,12)	1:668:C:SER:N	1:668:C:SER:CA	1:668:C:SER:C	1:669:C:LEU:N	4	1.08
(1,68)	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	1:701:C:VAL:N	7	1.07
(1,52)	1:692:C:LEU:N	1:692:C:LEU:CA	1:692:C:LEU:C	1:693:C:ILE:N	11	1.07
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	9	1.07
(1,64)	1:698:C:VAL:N	1:698:C:VAL:CA	1:698:C:VAL:C	1:699:C:PHE:N	12	1.06
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	4	1.06
(1,45)	1:687:C:ILE:C	1:688:C:ILE:N	1:688:C:ILE:CA	1:688:C:ILE:C	6	1.05
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	14	1.04
(1,40)	1:685:C:PHE:N	1:685:C:PHE:CA	1:685:C:PHE:C	1:686:C:ILE:N	12	1.04
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	10	1.04
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	9	1.02
(1,57)	1:694:C:GLY:C	1:695:C:LEU:N	1:695:C:LEU:CA	1:695:C:LEU:C	9	1.01
(1,68)	1:700:C:ALA:N	1:700:C:ALA:CA	1:700:C:ALA:C	1:701:C:VAL:N	13	1.0