



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:01 AM UTC

PDB ID : 9GEC / pdb_00009gec
BMRB ID : 34952
Title : Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR) at 299K
Authors : Horvath, D.
Deposited on : 2024-08-07

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

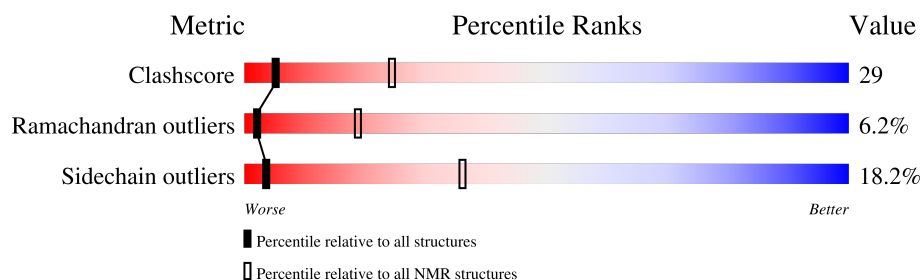
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 53%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	25	12% 32% 8% 48%

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:5-A:17 (13)	0.43	8

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

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

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

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 390 atoms, of which 193 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR).

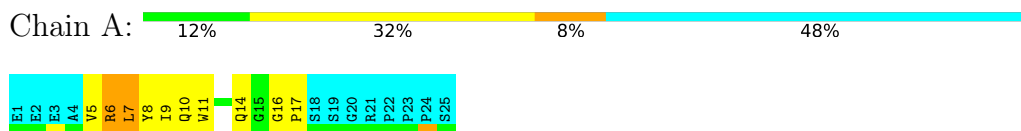
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	25	390	124	193	35	38	0

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)

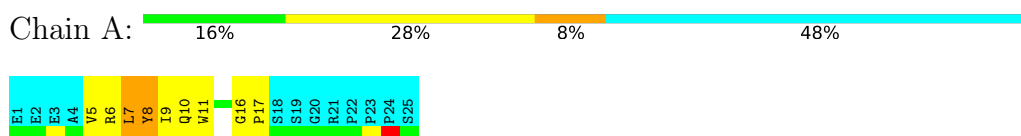


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

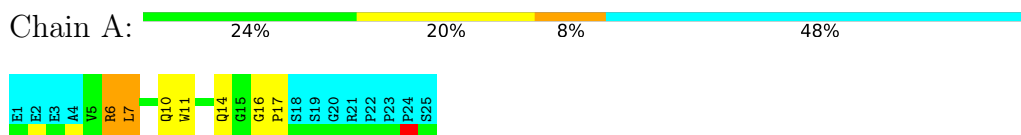
4.2.1 Score per residue for model 1

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



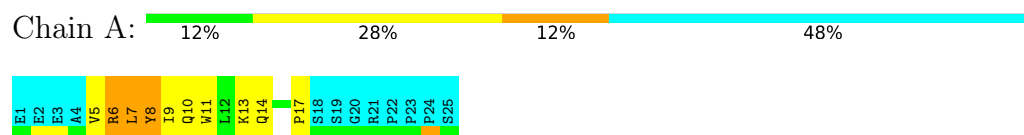
4.2.2 Score per residue for model 2

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



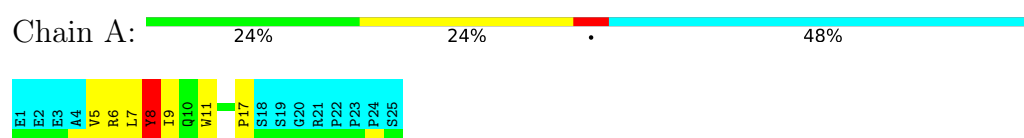
4.2.3 Score per residue for model 3

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



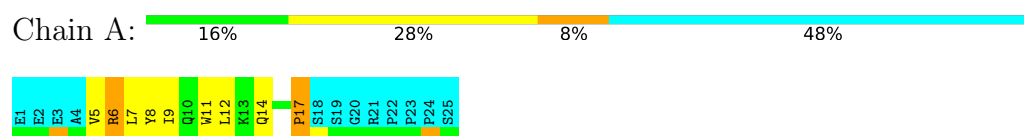
4.2.4 Score per residue for model 4

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



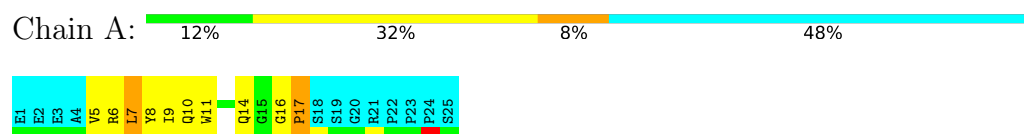
4.2.5 Score per residue for model 5

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



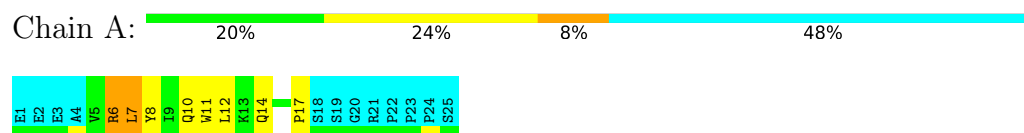
4.2.6 Score per residue for model 6

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



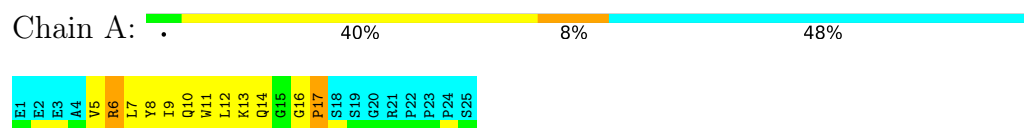
4.2.7 Score per residue for model 7

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



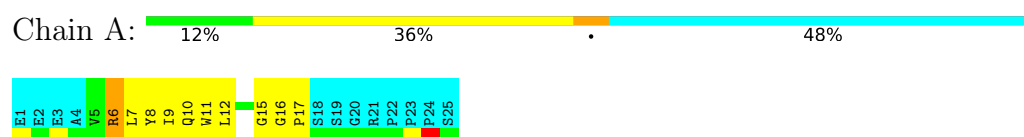
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



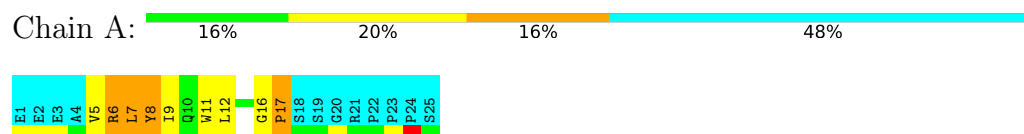
4.2.9 Score per residue for model 9

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



4.2.10 Score per residue for model 10

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CcpNmr Analysis Assign	refinement	2.4.1.
ARIA2alpha	structure calculation	2.3.1.

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	162
Number of shifts mapped to atoms	162
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	53%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.73±0.17	0±1/114 (0.2± 0.5%)	1.19±0.07	1±1/155 (0.4± 0.6%)
All	All	0.75	2/1140 (0.2%)	1.19	6/1550 (0.4%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	8	TYR	CE1-CZ	7.61	1.56	1.38	4	1
1	A	8	TYR	CE2-CZ	-7.31	1.20	1.38	4	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	16	GLY	CA-C-N	5.73	127.00	119.84	10	3
1	A	16	GLY	C-N-CA	5.73	127.00	119.84	10	3

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	110	116	116	6±2
All	All	1100	1160	1160	65

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:H	1:A:7:LEU:HD23	0.81	1.35	2	1
1:A:7:LEU:HD12	1:A:7:LEU:H	0.72	1.42	5	1
1:A:11:TRP:CH2	1:A:17:PRO:HD3	0.69	2.21	6	10
1:A:6:ARG:HG3	1:A:7:LEU:HD23	0.67	1.66	7	1
1:A:7:LEU:HD12	1:A:8:TYR:N	0.65	2.06	8	2
1:A:6:ARG:HD3	1:A:7:LEU:N	0.64	2.08	9	3
1:A:7:LEU:HD12	1:A:8:TYR:H	0.58	1.58	10	3
1:A:5:VAL:O	1:A:9:ILE:HG12	0.55	2.02	4	6
1:A:6:ARG:HG3	1:A:7:LEU:N	0.54	2.17	3	1
1:A:6:ARG:HG3	1:A:7:LEU:H	0.53	1.64	3	1
1:A:11:TRP:CZ2	1:A:17:PRO:HD3	0.51	2.40	9	5
1:A:10:GLN:O	1:A:14:GLN:HG3	0.49	2.07	2	3
1:A:11:TRP:O	1:A:14:GLN:HG2	0.47	2.09	5	1
1:A:7:LEU:CD1	1:A:8:TYR:H	0.47	2.21	10	1
1:A:8:TYR:O	1:A:11:TRP:HB3	0.47	2.09	7	5
1:A:7:LEU:H	1:A:7:LEU:CD2	0.46	2.17	2	1
1:A:8:TYR:CZ	1:A:12:LEU:HD11	0.45	2.47	7	3
1:A:7:LEU:HD12	1:A:7:LEU:N	0.45	2.26	1	2
1:A:7:LEU:HD23	1:A:7:LEU:N	0.45	2.16	2	1
1:A:7:LEU:N	1:A:7:LEU:HD12	0.44	2.27	3	1
1:A:10:GLN:O	1:A:14:GLN:HG2	0.44	2.12	7	2
1:A:5:VAL:HG13	1:A:6:ARG:N	0.43	2.29	4	1
1:A:5:VAL:O	1:A:8:TYR:HB3	0.42	2.14	5	1
1:A:6:ARG:O	1:A:10:GLN:HG2	0.42	2.15	9	1
1:A:8:TYR:CE1	1:A:12:LEU:HD11	0.42	2.50	5	2
1:A:5:VAL:O	1:A:8:TYR:HD1	0.42	1.98	4	1
1:A:9:ILE:O	1:A:13:LYS:HD3	0.41	2.16	8	1
1:A:7:LEU:O	1:A:10:GLN:HB2	0.41	2.15	1	1
1:A:7:LEU:H	1:A:7:LEU:CD1	0.41	2.23	5	1
1:A:7:LEU:CD1	1:A:8:TYR:N	0.41	2.84	10	1
1:A:9:ILE:O	1:A:13:LYS:HB2	0.40	2.16	3	1

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	13/25 (52%)	10±1 (76±11%)	2±1 (18±10%)	1±1 (6±5%)	2	19
All	All	130/250 (52%)	99 (76%)	23 (18%)	8 (6%)	2	19

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	17	PRO	4
1	A	16	GLY	3
1	A	15	GLY	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	11/21 (52%)	9±1 (82±6%)	2±1 (18±6%)	3	36
All	All	110/210 (52%)	90 (82%)	20 (18%)	3	36

All 4 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	6	ARG	8
1	A	7	LEU	6
1	A	8	TYR	4
1	A	9	ILE	2

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 53% for the well-defined parts and 48% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *nef_chemical_shift_list_ShiftList_1*

7.1.1 Bookkeeping

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

Total number of shifts	162
Number of shifts mapped to atoms	162
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

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

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 53%, i.e. 106 atoms were assigned a chemical shift out of a possible 201. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	27/65 (42%)	27/27 (100%)	0/26 (0%)	0/12 (0%)
Sidechain	70/115 (61%)	70/75 (93%)	0/34 (0%)	0/6 (0%)
Aromatic	9/21 (43%)	9/10 (90%)	0/10 (0%)	0/1 (0%)
Overall	106/201 (53%)	106/112 (95%)	0/70 (0%)	0/19 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 48%, i.e. 162 atoms were assigned a chemical shift out of a possible 335. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	46/120 (38%)	46/49 (94%)	0/50 (0%)	0/21 (0%)
Sidechain	107/194 (55%)	107/125 (86%)	0/60 (0%)	0/9 (0%)
Aromatic	9/21 (43%)	9/10 (90%)	0/10 (0%)	0/1 (0%)
Overall	162/335 (48%)	162/184 (88%)	0/120 (0%)	0/31 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

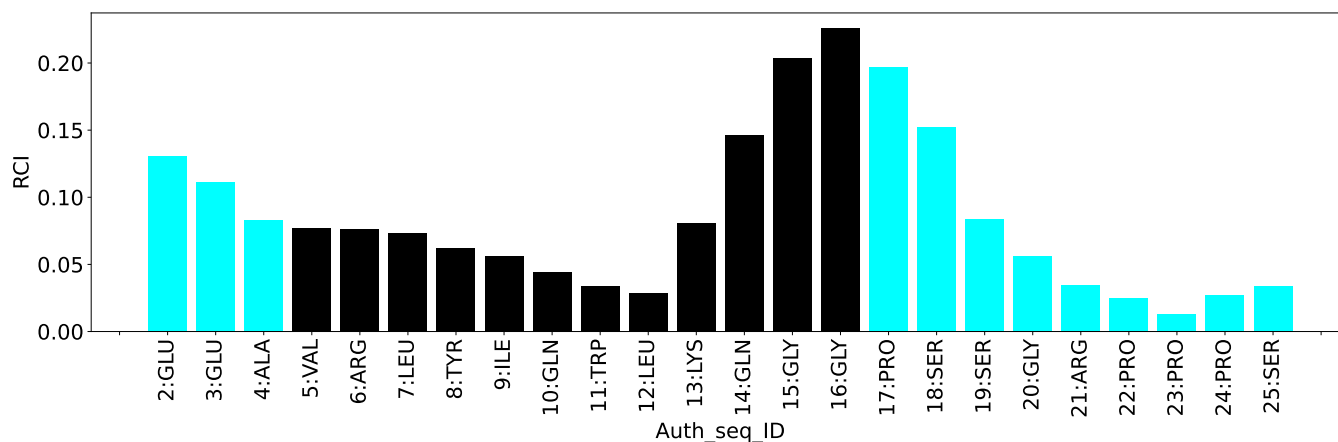
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	16	GLY	HA2	1.60	2.15 – 5.77	-6.5

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1020
Intra-residue ($ i-j =0$)	723
Sequential ($ i-j =1$)	147
Medium range ($ i-j >1$ and $ i-j <5$)	72
Long range ($ i-j \geq 5$)	78
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	40.8
Number of long range restraints per residue ¹	3.1

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)	50.0	0.2
0.2-0.5 (Medium)	80.5	0.5
>0.5 (Large)	117.1	4.43

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

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

9 Distance violation analysis ⓘ

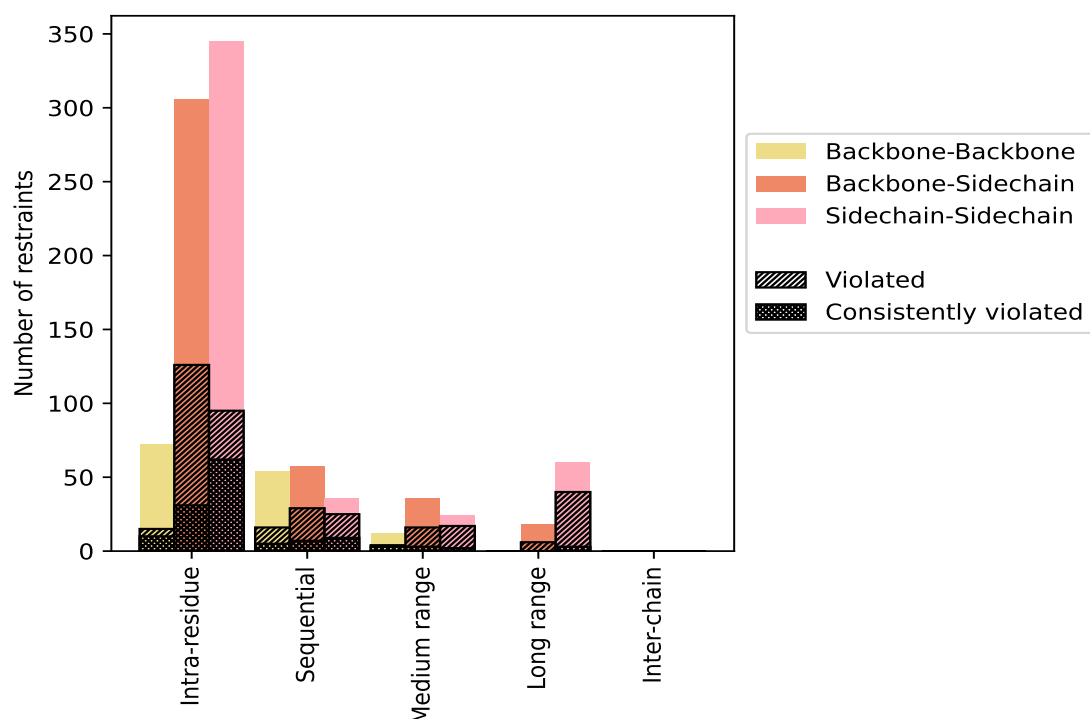
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	723	70.9	236	32.6	23.1	103	14.2	10.1
Backbone-Backbone	72	7.1	15	20.8	1.5	10	13.9	1.0
Backbone-Sidechain	306	30.0	126	41.2	12.4	31	10.1	3.0
Sidechain-Sidechain	345	33.8	95	27.5	9.3	62	18.0	6.1
Sequential ($i-j =1$)	147	14.4	70	47.6	6.9	21	14.3	2.1
Backbone-Backbone	54	5.3	16	29.6	1.6	5	9.3	0.5
Backbone-Sidechain	57	5.6	29	50.9	2.8	7	12.3	0.7
Sidechain-Sidechain	36	3.5	25	69.4	2.5	9	25.0	0.9
Medium range ($i-j >1$ & $i-j <5$)	72	7.1	37	51.4	3.6	8	11.1	0.8
Backbone-Backbone	12	1.2	4	33.3	0.4	3	25.0	0.3
Backbone-Sidechain	36	3.5	16	44.4	1.6	3	8.3	0.3
Sidechain-Sidechain	24	2.4	17	70.8	1.7	2	8.3	0.2
Long range ($i-j \geq 5$)	78	7.6	46	59.0	4.5	3	3.8	0.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	18	1.8	6	33.3	0.6	0	0.0	0.0
Sidechain-Sidechain	60	5.9	40	66.7	3.9	3	5.0	0.3
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1020	100.0	389	38.1	38.1	135	13.2	13.2
Backbone-Backbone	138	13.5	35	25.4	3.4	18	13.0	1.8
Backbone-Sidechain	417	40.9	177	42.4	17.4	41	9.8	4.0
Sidechain-Sidechain	465	45.6	177	38.1	17.4	76	16.3	7.5

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

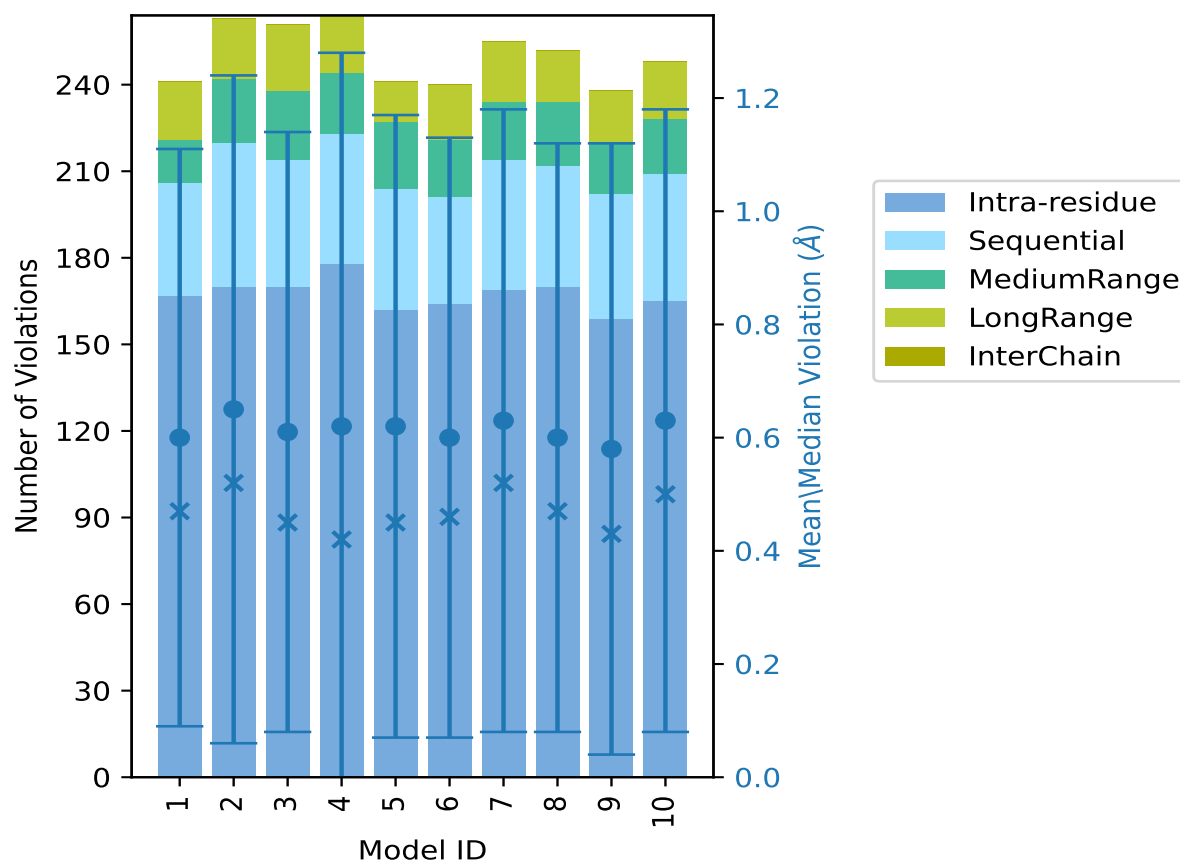
9.2 Distance violation statistics for each model [i](#)

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	167	39	15	20	0	241	0.6	4.04	0.51	0.47
2	170	50	22	21	0	263	0.65	4.08	0.59	0.52
3	170	44	24	23	0	261	0.61	4.27	0.53	0.45
4	178	45	21	20	0	264	0.62	4.43	0.66	0.42
5	162	42	23	14	0	241	0.62	4.09	0.55	0.45
6	164	37	20	19	0	240	0.6	4.03	0.53	0.46
7	169	45	20	21	0	255	0.63	4.07	0.55	0.52
8	170	42	22	18	0	252	0.6	4.08	0.52	0.47
9	159	43	18	18	0	238	0.58	4.06	0.54	0.43
10	165	44	19	20	0	248	0.63	4.26	0.55	0.5

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 631(IR:487, SQ:77, MR:35, LR:32, 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	%
32	11	6	12	0	61	1	10.0
9	13	0	9	0	31	2	20.0
12	1	3	8	0	24	3	30.0

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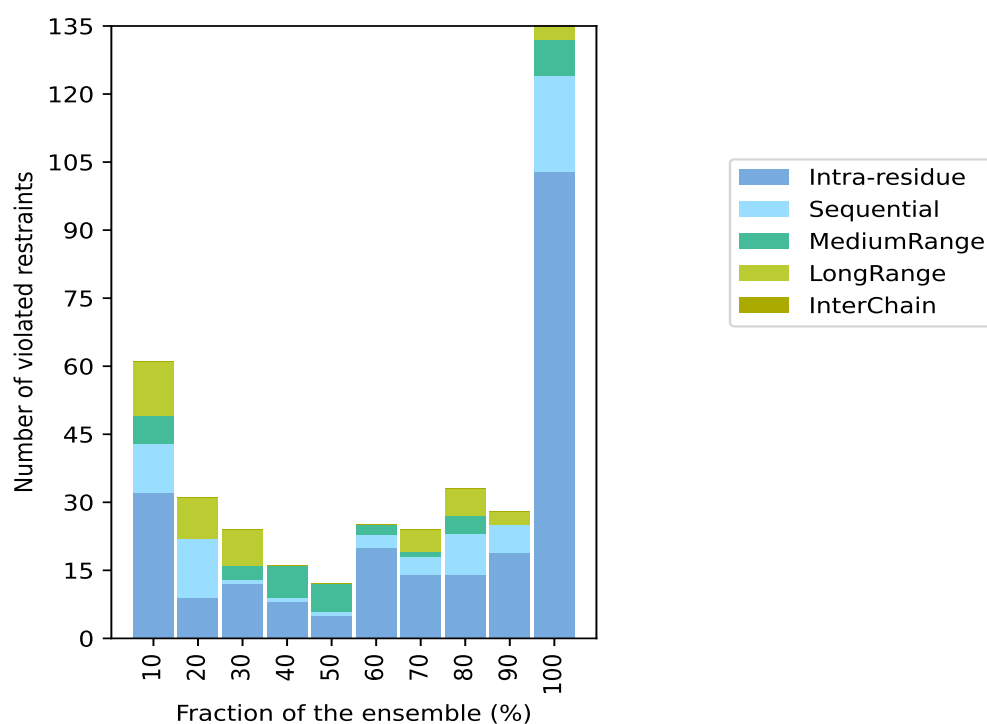
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
8	1	7	0	0	16	4	40.0
5	1	6	0	0	12	5	50.0
20	3	2	0	0	25	6	60.0
14	4	1	5	0	24	7	70.0
14	9	4	6	0	33	8	80.0
19	6	0	3	0	28	9	90.0
103	21	8	3	0	135	10	100.0

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

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

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

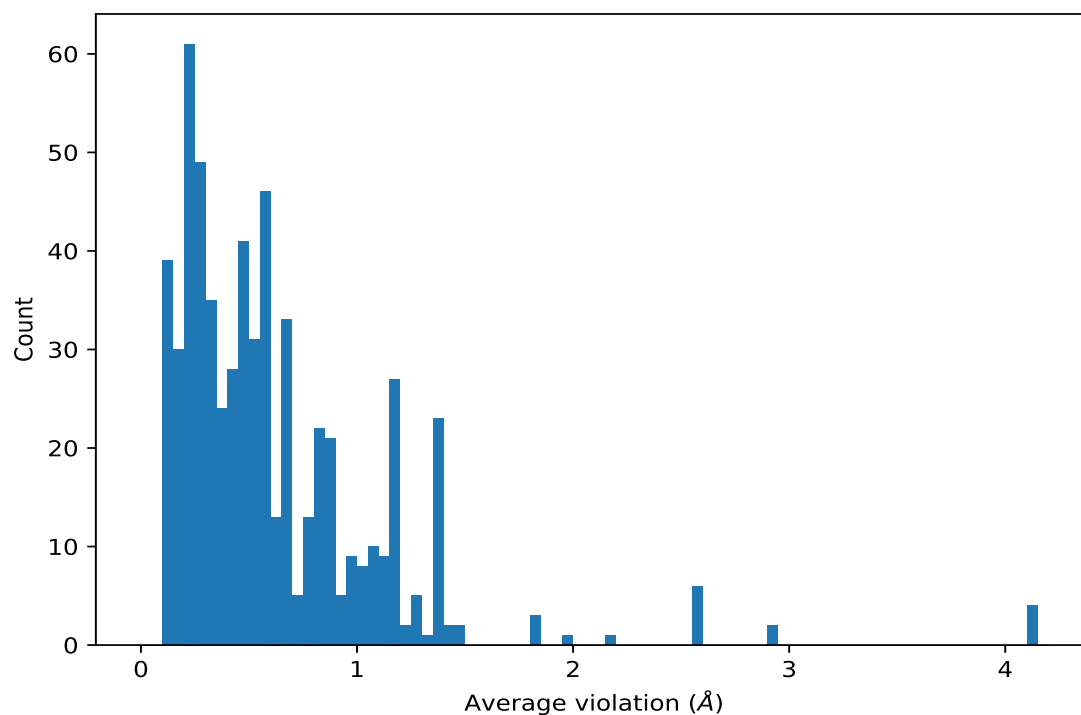


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	10	4.11	0.08	4.08
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	10	4.11	0.08	4.08
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	10	4.11	0.08	4.08
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	10	4.11	0.08	4.08
(2,234)	1:5:A:VAL:H	1:7:A:LEU:HA	10	2.92	0.31	3.06
(4,9)	1:5:A:VAL:H	1:7:A:LEU:HA	10	2.92	0.31	3.06
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	10	2.58	0.62	2.42
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	10	2.58	0.62	2.42
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	10	2.58	0.62	2.42
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	10	2.58	0.62	2.42
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	10	2.58	0.62	2.42
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	10	2.58	0.62	2.42
(1,234)	1:5:A:VAL:H	1:7:A:LEU:HA	10	2.18	0.31	2.32
(1,120)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	10	1.97	0.19	1.96
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	10	1.83	0.62	1.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	10	1.83	0.62	1.65
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	10	1.83	0.62	1.65
(2,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	10	1.49	0.41	1.64
(4,14)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	10	1.49	0.41	1.64
(2,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	10	1.4	0.93	1.4
(3,299)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	10	1.4	0.93	1.4
(2,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	1.37	0.33	1.49
(3,296)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	1.37	0.33	1.49
(1,268)	1:18:A:SER:H	1:18:A:SER:HA	10	1.32	0.04	1.33
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG2	10	1.27	0.11	1.31
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG3	10	1.27	0.11	1.31
(2,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	1.25	0.06	1.26
(4,2)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	1.25	0.06	1.26
(1,180)	1:9:A:ILE:HB	1:9:A:ILE:HG13	10	1.25	0.07	1.2
(1,21)	1:15:A:GLY:H	1:15:A:GLY:HA2	10	1.24	0.2	1.33
(1,73)	1:23:A:PRO:HA	1:23:A:PRO:HG2	10	1.2	0.03	1.2
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	1.18	0.03	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	10	1.18	0.03	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	10	1.18	0.03	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	10	1.18	0.03	1.19
(1,199)	1:12:A:LEU:HA	1:12:A:LEU:HG	10	1.17	0.2	1.24
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD2	10	1.14	0.89	1.02
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD3	10	1.14	0.89	1.02
(1,267)	1:18:A:SER:H	1:18:A:SER:HB2	10	1.1	0.3	1.23
(1,267)	1:18:A:SER:H	1:18:A:SER:HB3	10	1.1	0.3	1.23
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	10	1.08	0.05	1.08
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	10	1.08	0.05	1.08
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	10	1.08	0.05	1.08
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	10	1.08	0.05	1.08
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	10	1.04	0.2	1.11
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	10	1.04	0.2	1.11
(1,158)	1:7:A:LEU:HB3	1:7:A:LEU:HG	10	1.03	0.26	1.15
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	1.03	0.05	1.02
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	1.03	0.05	1.02
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	10	1.03	0.05	1.02
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	10	1.03	0.05	1.02
(1,18)	1:19:A:SER:H	1:19:A:SER:HA	10	0.96	0.3	0.77
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	10	0.9	0.33	0.8
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	10	0.9	0.33	0.8
(1,309)	1:9:A:ILE:HA	1:12:A:LEU:HB2	10	0.89	0.05	0.89
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	10	0.88	0.03	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	10	0.88	0.03	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	10	0.88	0.03	0.9
(1,70)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.88	0.01	0.88
(1,291)	1:21:A:ARG:HA	1:22:A:PRO:HD2	10	0.87	0.19	0.93
(1,89)	1:24:A:PRO:HA	1:24:A:PRO:HB3	10	0.87	0.05	0.85
(1,84)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.8	0.03	0.82
(1,206)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.76	0.01	0.76
(1,206)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.76	0.01	0.76
(1,206)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.76	0.01	0.76
(2,221)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.76	0.01	0.76
(3,214)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.76	0.01	0.76
(1,16)	1:8:A:TYR:H	1:8:A:TYR:HB3	10	0.69	0.06	0.68
(1,24)	1:25:A:SER:H	1:25:A:SER:HB2	10	0.69	0.12	0.71
(1,24)	1:25:A:SER:H	1:25:A:SER:HB3	10	0.69	0.12	0.71
(1,31)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.68	0.02	0.69
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	10	0.68	0.02	0.68
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	10	0.68	0.02	0.68
(1,67)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	10	0.68	0.01	0.68
(1,67)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.68	0.01	0.68
(1,284)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	10	0.66	0.29	0.58
(1,72)	1:23:A:PRO:HA	1:23:A:PRO:HG3	10	0.66	0.27	0.58
(1,222)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	0.65	0.01	0.65
(1,224)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.65	0.0	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	10	0.65	0.01	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	10	0.65	0.01	0.65
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.63	0.01	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	10	0.63	0.01	0.63
(1,66)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.63	0.02	0.62
(1,66)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	10	0.63	0.02	0.62
(1,225)	1:16:A:GLY:H	1:16:A:GLY:HA3	10	0.62	0.02	0.63
(1,55)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.62	0.02	0.63
(1,38)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.62	0.0	0.62
(1,78)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	10	0.62	0.01	0.62
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	10	0.61	0.08	0.57
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	10	0.61	0.08	0.57
(2,218)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.6	0.01	0.6
(3,211)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.6	0.01	0.6
(1,171)	1:9:A:ILE:HA	1:9:A:ILE:HG12	10	0.6	0.49	0.24
(1,79)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.6	0.0	0.6
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD2	10	0.59	0.16	0.66
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD3	10	0.59	0.16	0.66
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	10	0.59	0.23	0.57
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	10	0.59	0.23	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	10	0.59	0.23	0.57
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	10	0.59	0.23	0.57
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	10	0.59	0.23	0.57
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	10	0.59	0.23	0.57
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	10	0.59	0.23	0.57
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	10	0.59	0.23	0.57
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	10	0.59	0.23	0.57
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	10	0.59	0.23	0.57
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	10	0.59	0.23	0.57
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	10	0.59	0.23	0.57
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	10	0.59	0.1	0.61
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	10	0.59	0.1	0.61
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	10	0.59	0.1	0.61
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	10	0.59	0.1	0.61
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD2	10	0.57	0.04	0.57
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.57	0.04	0.57
(1,119)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	10	0.57	0.24	0.67
(1,205)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.57	0.0	0.57
(1,205)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.57	0.0	0.57
(1,205)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.57	0.0	0.57
(1,141)	1:7:A:LEU:H	1:8:A:TYR:H	10	0.55	0.14	0.56
(2,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	10	0.54	0.34	0.42
(4,15)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	10	0.54	0.34	0.42
(1,231)	1:11:A:TRP:HB3	1:12:A:LEU:H	10	0.53	0.04	0.54
(1,5)	1:4:A:ALA:H	1:4:A:ALA:HA	10	0.52	0.01	0.52
(1,87)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	10	0.52	0.09	0.5
(1,162)	1:7:A:LEU:HD21	1:7:A:LEU:HG	10	0.51	0.03	0.52
(1,162)	1:7:A:LEU:HD22	1:7:A:LEU:HG	10	0.51	0.03	0.52
(1,162)	1:7:A:LEU:HD23	1:7:A:LEU:HG	10	0.51	0.03	0.52
(1,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.51	0.05	0.52
(1,118)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.5	0.27	0.34
(1,71)	1:23:A:PRO:HA	1:23:A:PRO:HB2	10	0.5	0.06	0.51
(1,86)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.48	0.05	0.51
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB2	10	0.48	0.09	0.44
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB3	10	0.48	0.09	0.44
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	10	0.48	0.12	0.46
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	10	0.48	0.12	0.46
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	10	0.48	0.12	0.46
(1,113)	1:6:A:ARG:HA	1:6:A:ARG:HB2	10	0.47	0.14	0.44
(1,198)	1:12:A:LEU:HA	1:12:A:LEU:HB3	10	0.45	0.02	0.44
(1,4)	1:3:A:GLU:H	1:3:A:GLU:HA	10	0.44	0.04	0.44
(1,64)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.43	0.0	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,157)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.42	0.01	0.42
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	10	0.42	0.01	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.42	0.01	0.41
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.41	0.02	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	10	0.41	0.02	0.42
(1,290)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	10	0.41	0.03	0.42
(1,74)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.4	0.01	0.41
(2,293)	1:8:A:TYR:HA	1:11:A:TRP:HB2	10	0.4	0.07	0.44
(3,280)	1:8:A:TYR:HA	1:11:A:TRP:HB2	10	0.4	0.07	0.44
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	10	0.38	0.0	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	10	0.38	0.0	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	10	0.38	0.0	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	10	0.38	0.0	0.38
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	10	0.38	0.1	0.39
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	10	0.38	0.1	0.39
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	10	0.38	0.1	0.39
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	10	0.38	0.1	0.39
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	10	0.38	0.1	0.39
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	10	0.38	0.1	0.39
(1,23)	1:25:A:SER:H	1:25:A:SER:HA	10	0.37	0.02	0.37
(2,28)	1:17:A:PRO:HA	1:17:A:PRO:HD2	10	0.37	0.05	0.39
(4,1)	1:17:A:PRO:HA	1:17:A:PRO:HD2	10	0.37	0.05	0.39
(1,47)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	10	0.36	0.01	0.36
(1,122)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.35	0.01	0.35
(1,185)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	10	0.34	0.01	0.33
(1,185)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	10	0.34	0.01	0.33
(1,185)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	10	0.34	0.01	0.33
(1,25)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.32	0.0	0.32
(1,194)	1:20:A:GLY:H	1:20:A:GLY:HA3	10	0.31	0.17	0.22
(1,140)	1:11:A:TRP:H	1:12:A:LEU:H	10	0.3	0.07	0.28
(1,133)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	10	0.3	0.02	0.3
(1,133)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	10	0.3	0.02	0.3
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB2	10	0.3	0.04	0.3
(2,232)	1:7:A:LEU:H	1:8:A:TYR:HB3	10	0.29	0.08	0.29
(4,8)	1:7:A:LEU:H	1:8:A:TYR:HB3	10	0.29	0.08	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG11	10	0.29	0.01	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG12	10	0.29	0.01	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG13	10	0.29	0.01	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG21	10	0.29	0.01	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG22	10	0.29	0.01	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG23	10	0.29	0.01	0.29
(1,181)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	10	0.29	0.0	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,275)	1:9:A:ILE:H	1:10:A:GLN:H	10	0.29	0.04	0.29
(2,230)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.28	0.02	0.28
(3,223)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.28	0.02	0.28
(1,131)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	10	0.28	0.0	0.28
(1,316)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	10	0.28	0.01	0.28
(1,2)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	10	0.27	0.0	0.27
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG2	10	0.26	0.1	0.22
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG3	10	0.26	0.1	0.22
(1,197)	1:12:A:LEU:HA	1:12:A:LEU:HB2	10	0.25	0.01	0.24
(1,317)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	10	0.24	0.03	0.24
(1,159)	1:7:A:LEU:HD11	1:7:A:LEU:HG	10	0.2	0.01	0.2
(1,159)	1:7:A:LEU:HD12	1:7:A:LEU:HG	10	0.2	0.01	0.2
(1,159)	1:7:A:LEU:HD13	1:7:A:LEU:HG	10	0.2	0.01	0.2
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB2	10	0.18	0.02	0.18
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB3	10	0.18	0.02	0.18
(1,96)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.18	0.0	0.18
(2,265)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	10	0.18	0.0	0.18
(4,13)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	10	0.18	0.0	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	10	0.17	0.02	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	10	0.17	0.02	0.18
(2,95)	1:11:A:TRP:HA	1:11:A:TRP:HB3	10	0.16	0.0	0.16
(3,90)	1:11:A:TRP:HA	1:11:A:TRP:HB3	10	0.16	0.0	0.16
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG21	10	0.15	0.0	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG22	10	0.15	0.0	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG23	10	0.15	0.0	0.15
(1,3)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	10	0.14	0.0	0.14
(2,278)	1:10:A:GLN:H	1:11:A:TRP:H	10	0.14	0.02	0.14
(3,265)	1:10:A:GLN:H	1:11:A:TRP:H	10	0.14	0.02	0.14
(1,201)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.13	0.0	0.13
(1,26)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.12	0.0	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.12	0.01	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.12	0.01	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.12	0.01	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.12	0.01	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.12	0.01	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.12	0.01	0.12
(1,187)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	10	0.11	0.0	0.11
(1,187)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	10	0.11	0.0	0.11
(1,187)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	10	0.11	0.0	0.11
(1,75)	1:23:A:PRO:HG2	1:23:A:PRO:HG3	10	0.1	0.0	0.1
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	9	1.11	0.01	1.11
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	9	1.11	0.01	1.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	9	1.11	0.01	1.11
(1,117)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	9	1.11	0.44	1.11
(1,288)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	9	0.97	0.15	0.9
(1,288)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	9	0.97	0.15	0.9
(1,61)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	9	0.9	0.04	0.91
(1,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	9	0.89	0.16	0.93
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.89	0.37	1.17
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.89	0.37	1.17
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.89	0.37	1.17
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.89	0.37	1.17
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.89	0.37	1.17
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.89	0.37	1.17
(1,313)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	9	0.86	0.32	1.06
(1,80)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	9	0.81	0.23	0.84
(1,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.73	0.09	0.75
(1,279)	1:19:A:SER:H	1:20:A:GLY:H	9	0.68	0.26	0.85
(1,286)	1:21:A:ARG:H	1:21:A:ARG:HB2	9	0.61	0.13	0.64
(1,139)	1:5:A:VAL:H	1:6:A:ARG:H	9	0.59	0.31	0.62
(1,223)	1:15:A:GLY:H	1:16:A:GLY:H	9	0.56	0.22	0.48
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.49	0.29	0.26
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.49	0.29	0.26
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.49	0.29	0.26
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.49	0.29	0.26
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.49	0.29	0.26
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.49	0.29	0.26
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG11	9	0.48	0.12	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG12	9	0.48	0.12	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG13	9	0.48	0.12	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG21	9	0.48	0.12	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG22	9	0.48	0.12	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG23	9	0.48	0.12	0.43
(1,44)	1:21:A:ARG:HA	1:21:A:ARG:HB3	9	0.43	0.1	0.45
(1,115)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	9	0.43	0.22	0.38
(1,281)	1:11:A:TRP:HE3	1:12:A:LEU:H	9	0.34	0.12	0.38
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	9	0.24	0.06	0.26
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	9	0.24	0.06	0.26
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	9	0.24	0.06	0.26
(2,240)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.23	0.02	0.23
(4,10)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.23	0.02	0.23
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	9	0.2	0.0	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	9	0.2	0.0	0.2
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	9	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	9	0.16	0.03	0.16
(1,13)	1:12:A:LEU:H	1:12:A:LEU:HA	9	0.13	0.01	0.14
(2,56)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	9	0.12	0.01	0.12
(3,53)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	9	0.12	0.01	0.12
(2,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	8	1.44	0.37	1.37
(3,306)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	8	1.44	0.37	1.37
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	8	1.39	0.11	1.42
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	8	1.39	0.11	1.42
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	8	1.39	0.11	1.42
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	8	1.39	0.11	1.42
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	8	1.39	0.11	1.42
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	8	1.39	0.11	1.42
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	8	1.39	0.11	1.42
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	8	1.39	0.11	1.42
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	8	1.39	0.11	1.42
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	8	1.39	0.11	1.42
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	8	1.39	0.11	1.42
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	8	1.39	0.11	1.42
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	8	1.39	0.11	1.42
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	8	1.39	0.11	1.42
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	8	1.39	0.11	1.42
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	8	1.39	0.11	1.42
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	8	1.39	0.11	1.42
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	8	1.39	0.11	1.42
(1,91)	1:24:A:PRO:HA	1:24:A:PRO:HG3	8	1.24	0.24	1.27
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	8	1.16	0.37	1.25
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	8	1.16	0.37	1.25
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	8	1.16	0.37	1.25
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	8	1.16	0.37	1.25
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	8	1.16	0.37	1.25
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	8	1.16	0.37	1.25
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	8	1.16	0.37	1.25
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	8	1.16	0.37	1.25
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	8	1.16	0.37	1.25
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	8	1.16	0.37	1.25
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	8	1.16	0.37	1.25
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	8	1.16	0.37	1.25
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	8	1.16	0.37	1.25
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	8	1.16	0.37	1.25
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	8	1.16	0.37	1.25
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	8	1.16	0.37	1.25
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	8	1.16	0.37	1.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	8	1.16	0.37	1.25
(1,252)	1:5:A:VAL:HG11	1:6:A:ARG:H	8	1.07	0.13	1.12
(1,252)	1:5:A:VAL:HG12	1:6:A:ARG:H	8	1.07	0.13	1.12
(1,252)	1:5:A:VAL:HG13	1:6:A:ARG:H	8	1.07	0.13	1.12
(1,252)	1:5:A:VAL:HG21	1:6:A:ARG:H	8	1.07	0.13	1.12
(1,252)	1:5:A:VAL:HG22	1:6:A:ARG:H	8	1.07	0.13	1.12
(1,252)	1:5:A:VAL:HG23	1:6:A:ARG:H	8	1.07	0.13	1.12
(1,320)	1:16:A:GLY:HA2	1:21:A:ARG:HB2	8	0.82	0.11	0.84
(1,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	8	0.73	0.31	0.62
(1,315)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	8	0.73	0.18	0.7
(2,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	8	0.67	0.25	0.68
(2,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	8	0.67	0.25	0.68
(3,247)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	8	0.67	0.25	0.68
(3,247)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	8	0.67	0.25	0.68
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	8	0.66	0.22	0.68
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	8	0.66	0.22	0.68
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	8	0.66	0.22	0.68
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	8	0.66	0.22	0.68
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	8	0.66	0.22	0.68
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	8	0.66	0.22	0.68
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	8	0.66	0.22	0.68
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	8	0.66	0.22	0.68
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	8	0.66	0.22	0.68
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	8	0.66	0.22	0.68
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	8	0.66	0.22	0.68
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	8	0.66	0.22	0.68
(1,273)	1:13:A:LYS:H	1:14:A:GLN:H	8	0.63	0.14	0.59
(1,165)	1:7:A:LEU:H	1:7:A:LEU:HG	8	0.6	0.07	0.6
(1,260)	1:4:A:ALA:HB1	1:5:A:VAL:H	8	0.59	0.24	0.58
(1,260)	1:4:A:ALA:HB2	1:5:A:VAL:H	8	0.59	0.24	0.58
(1,260)	1:4:A:ALA:HB3	1:5:A:VAL:H	8	0.59	0.24	0.58
(1,145)	1:5:A:VAL:HA	1:5:A:VAL:HB	8	0.59	0.04	0.58
(2,166)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.54	0.09	0.5
(3,159)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.54	0.09	0.5
(1,129)	1:14:A:GLN:HA	1:14:A:GLN:HG2	8	0.52	0.23	0.62
(1,121)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	8	0.52	0.11	0.59
(1,109)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.49	0.3	0.48
(2,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	8	0.42	0.4	0.2
(4,4)	1:24:A:PRO:HA	1:24:A:PRO:HD3	8	0.42	0.4	0.2
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB2	8	0.33	0.11	0.38
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB3	8	0.33	0.11	0.38
(2,248)	1:5:A:VAL:HB	1:6:A:ARG:H	8	0.25	0.04	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,237)	1:5:A:VAL:HB	1:6:A:ARG:H	8	0.25	0.04	0.26
(1,137)	1:24:A:PRO:HA	1:25:A:SER:H	8	0.21	0.04	0.22
(1,57)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	8	0.2	0.01	0.2
(1,152)	1:7:A:LEU:HA	1:7:A:LEU:HB2	8	0.18	0.08	0.14
(1,192)	1:11:A:TRP:H	1:11:A:TRP:HB3	8	0.13	0.01	0.13
(1,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	7	1.14	0.64	0.84
(1,110)	1:6:A:ARG:H	1:6:A:ARG:HG3	7	0.9	0.58	0.72
(1,329)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	7	0.81	0.2	0.95
(1,329)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	7	0.81	0.2	0.95
(1,329)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	7	0.81	0.2	0.95
(1,247)	1:21:A:ARG:H	1:21:A:ARG:HG2	7	0.71	0.21	0.66
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG2	7	0.54	0.17	0.57
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG3	7	0.54	0.17	0.57
(1,193)	1:20:A:GLY:H	1:20:A:GLY:HA2	7	0.52	0.01	0.52
(1,304)	1:3:A:GLU:HA	1:6:A:ARG:HB3	7	0.48	0.22	0.49
(2,242)	1:6:A:ARG:HB3	1:7:A:LEU:H	7	0.42	0.25	0.49
(3,232)	1:6:A:ARG:HB3	1:7:A:LEU:H	7	0.42	0.25	0.49
(1,296)	1:8:A:TYR:HA	1:24:A:PRO:HD3	7	0.4	0.17	0.37
(1,283)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	7	0.37	0.32	0.18
(1,112)	1:6:A:ARG:HA	1:6:A:ARG:HB3	7	0.36	0.15	0.44
(1,7)	1:3:A:GLU:HA	1:4:A:ALA:H	7	0.35	0.09	0.36
(1,255)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	7	0.33	0.2	0.26
(1,255)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	7	0.33	0.2	0.26
(2,51)	1:22:A:PRO:HA	1:22:A:PRO:HD3	7	0.32	0.3	0.14
(4,3)	1:22:A:PRO:HA	1:22:A:PRO:HD3	7	0.32	0.3	0.14
(2,108)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.27	0.13	0.36
(3,103)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.27	0.13	0.36
(1,125)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	7	0.21	0.02	0.21
(2,322)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	7	0.16	0.02	0.17
(3,307)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	7	0.16	0.02	0.17
(1,298)	1:8:A:TYR:HA	1:8:A:TYR:HB2	7	0.14	0.03	0.14
(2,92)	1:24:A:PRO:HA	1:24:A:PRO:HD2	7	0.14	0.05	0.11
(3,89)	1:24:A:PRO:HA	1:24:A:PRO:HD2	7	0.14	0.05	0.11
(1,337)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	6	0.85	0.34	0.92
(1,337)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	6	0.85	0.34	0.92
(1,337)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	6	0.85	0.34	0.92
(1,104)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.74	0.1	0.72
(1,269)	1:19:A:SER:H	1:19:A:SER:HB2	6	0.7	0.16	0.72
(1,239)	1:3:A:GLU:HB3	1:4:A:ALA:H	6	0.66	0.23	0.6
(1,176)	1:9:A:ILE:H	1:9:A:ILE:HG12	6	0.61	0.03	0.61
(1,134)	1:14:A:GLN:H	1:14:A:GLN:HG3	6	0.54	0.17	0.57
(1,98)	1:10:A:GLN:HA	1:10:A:GLN:HG2	6	0.51	0.04	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	6	0.49	0.03	0.48
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	6	0.49	0.03	0.48
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	6	0.49	0.03	0.48
(1,335)	1:7:A:LEU:HD11	1:8:A:TYR:HB2	6	0.48	0.25	0.53
(1,335)	1:7:A:LEU:HD12	1:8:A:TYR:HB2	6	0.48	0.25	0.53
(1,335)	1:7:A:LEU:HD13	1:8:A:TYR:HB2	6	0.48	0.25	0.53
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	6	0.47	0.11	0.5
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	6	0.47	0.11	0.5
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	6	0.47	0.11	0.5
(1,148)	1:3:A:GLU:HA	1:3:A:GLU:HB2	6	0.45	0.11	0.4
(1,238)	1:3:A:GLU:H	1:3:A:GLU:HB2	6	0.45	0.12	0.44
(1,149)	1:3:A:GLU:HA	1:3:A:GLU:HB3	6	0.44	0.07	0.46
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.4	0.09	0.44
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.4	0.09	0.44
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.4	0.09	0.44
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB2	6	0.35	0.19	0.28
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB3	6	0.35	0.19	0.28
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	6	0.29	0.01	0.29
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	6	0.29	0.01	0.29
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	6	0.29	0.01	0.29
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.27	0.08	0.28
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.27	0.08	0.28
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.27	0.08	0.28
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.27	0.08	0.28
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.27	0.08	0.28
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.27	0.08	0.28
(1,130)	1:14:A:GLN:HA	1:14:A:GLN:HG3	6	0.25	0.08	0.26
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	6	0.25	0.04	0.27
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	6	0.25	0.04	0.27
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	6	0.25	0.04	0.27
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	6	0.25	0.04	0.27
(1,297)	1:8:A:TYR:HA	1:11:A:TRP:HB3	6	0.25	0.13	0.22
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB2	6	0.23	0.07	0.22
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB3	6	0.23	0.07	0.22
(2,246)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.23	0.11	0.21
(3,235)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.23	0.11	0.21
(1,14)	1:8:A:TYR:H	1:8:A:TYR:HA	6	0.13	0.02	0.12
(2,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	5	0.99	0.64	1.37
(2,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	5	0.99	0.64	1.37
(2,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	5	0.99	0.64	1.37
(3,312)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	5	0.99	0.64	1.37
(3,312)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	5	0.99	0.64	1.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,312)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	5	0.99	0.64	1.37
(1,114)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	5	0.94	0.65	0.77
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD11	5	0.81	0.34	0.96
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD12	5	0.81	0.34	0.96
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD13	5	0.81	0.34	0.96
(1,270)	1:19:A:SER:H	1:19:A:SER:HB3	5	0.8	0.29	1.0
(1,20)	1:2:A:GLU:HA	1:3:A:GLU:H	5	0.48	0.13	0.5
(1,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	5	0.31	0.05	0.3
(1,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	5	0.31	0.05	0.3
(1,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	5	0.31	0.05	0.3
(1,327)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	5	0.31	0.05	0.3
(1,327)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	5	0.31	0.05	0.3
(1,327)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	5	0.31	0.05	0.3
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	5	0.21	0.07	0.22
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	5	0.21	0.07	0.22
(1,154)	1:7:A:LEU:HA	1:7:A:LEU:HB3	5	0.14	0.02	0.14
(1,226)	1:16:A:GLY:H	1:16:A:GLY:HA2	5	0.13	0.01	0.13
(2,308)	1:9:A:ILE:HA	1:12:A:LEU:HB3	5	0.11	0.01	0.11
(3,294)	1:9:A:ILE:HA	1:12:A:LEU:HB3	5	0.11	0.01	0.11
(1,106)	1:6:A:ARG:HA	1:6:A:ARG:HG2	4	1.38	0.73	1.64
(1,324)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	4	0.89	0.18	0.92
(1,324)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	4	0.89	0.18	0.92
(1,324)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	4	0.89	0.18	0.92
(1,324)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	4	0.89	0.18	0.92
(1,324)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	4	0.89	0.18	0.92
(1,324)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	4	0.89	0.18	0.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,334)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	4	0.79	0.26	0.73
(1,334)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	4	0.79	0.26	0.73
(1,334)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	4	0.79	0.26	0.73
(1,334)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	4	0.79	0.26	0.73
(1,334)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	4	0.79	0.26	0.73
(1,334)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	4	0.79	0.26	0.73
(1,103)	1:10:A:GLN:H	1:10:A:GLN:HG2	4	0.57	0.06	0.57
(1,326)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	4	0.55	0.24	0.5
(1,326)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	4	0.55	0.24	0.5
(1,326)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	4	0.55	0.24	0.5
(1,326)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	4	0.55	0.24	0.5
(1,326)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	4	0.55	0.24	0.5
(1,326)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	4	0.55	0.24	0.5
(1,135)	1:14:A:GLN:H	1:14:A:GLN:HG2	4	0.44	0.19	0.38
(1,177)	1:9:A:ILE:H	1:9:A:ILE:HG13	4	0.43	0.11	0.44
(2,135)	1:14:A:GLN:H	1:14:A:GLN:HG2	4	0.26	0.13	0.19
(3,130)	1:14:A:GLN:H	1:14:A:GLN:HG2	4	0.26	0.13	0.19
(2,303)	1:3:A:GLU:HA	1:6:A:ARG:HB2	4	0.22	0.04	0.24
(3,289)	1:3:A:GLU:HA	1:6:A:ARG:HB2	4	0.22	0.04	0.24
(1,244)	1:12:A:LEU:HB2	1:13:A:LYS:H	4	0.22	0.09	0.17
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD21	4	0.2	0.1	0.17
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD22	4	0.2	0.1	0.17
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD23	4	0.2	0.1	0.17
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD21	4	0.2	0.1	0.17
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD22	4	0.2	0.1	0.17
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD23	4	0.2	0.1	0.17
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.18	0.03	0.18
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.18	0.03	0.18
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.18	0.03	0.18
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.18	0.03	0.18
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.18	0.03	0.18
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.18	0.03	0.18
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD21	3	1.2	0.13	1.21
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD22	3	1.2	0.13	1.21
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD23	3	1.2	0.13	1.21
(1,285)	1:3:A:GLU:HB2	1:4:A:ALA:H	3	1.03	0.14	1.1
(2,272)	1:19:A:SER:HA	1:19:A:SER:HB3	3	0.55	0.0	0.55
(3,259)	1:19:A:SER:HA	1:19:A:SER:HB3	3	0.55	0.0	0.55
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD11	3	0.54	0.27	0.67
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD12	3	0.54	0.27	0.67
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD13	3	0.54	0.27	0.67
(2,332)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	3	0.52	0.08	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,332)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	3	0.52	0.08	0.47
(2,332)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	3	0.52	0.08	0.47
(3,317)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	3	0.52	0.08	0.47
(3,317)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	3	0.52	0.08	0.47
(3,317)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	3	0.52	0.08	0.47
(2,331)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	3	0.47	0.22	0.6
(2,331)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	3	0.47	0.22	0.6
(2,331)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	3	0.47	0.22	0.6
(3,316)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	3	0.47	0.22	0.6
(3,316)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	3	0.47	0.22	0.6
(3,316)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	3	0.47	0.22	0.6
(2,324)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	3	0.39	0.04	0.4
(2,324)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	3	0.39	0.04	0.4
(2,324)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	3	0.39	0.04	0.4
(3,309)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	3	0.39	0.04	0.4
(3,309)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	3	0.39	0.04	0.4
(3,309)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	3	0.39	0.04	0.4
(2,330)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	3	0.33	0.2	0.2
(2,330)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	3	0.33	0.2	0.2
(2,330)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	3	0.33	0.2	0.2
(3,315)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	3	0.33	0.2	0.2
(3,315)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	3	0.33	0.2	0.2
(3,315)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	3	0.33	0.2	0.2
(1,123)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	3	0.29	0.04	0.28
(1,150)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	3	0.22	0.08	0.27
(1,150)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	3	0.22	0.08	0.27
(2,111)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.21	0.07	0.26
(3,106)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.21	0.07	0.26
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	3	0.2	0.08	0.19
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	3	0.2	0.08	0.19
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	3	0.2	0.08	0.19
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG11	3	0.2	0.05	0.22
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG12	3	0.2	0.05	0.22
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG13	3	0.2	0.05	0.22
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG21	3	0.2	0.05	0.22
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG22	3	0.2	0.05	0.22
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG23	3	0.2	0.05	0.22
(1,46)	1:21:A:ARG:HA	1:21:A:ARG:HG2	3	0.19	0.1	0.14
(1,46)	1:21:A:ARG:HA	1:21:A:ARG:HG3	3	0.19	0.1	0.14
(1,124)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	3	0.15	0.02	0.14
(2,220)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	3	0.12	0.0	0.12
(3,213)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	3	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,151)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	3	0.1	0.0	0.1
(1,151)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	3	0.1	0.0	0.1
(1,332)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	2	0.85	0.12	0.85
(1,332)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	2	0.85	0.12	0.85
(1,332)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	2	0.85	0.12	0.85
(2,337)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	2	0.8	0.68	0.8
(2,337)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	2	0.8	0.68	0.8
(2,337)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	2	0.8	0.68	0.8
(3,322)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	2	0.8	0.68	0.8
(3,322)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	2	0.8	0.68	0.8
(3,322)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	2	0.8	0.68	0.8
(1,116)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	2	0.77	0.14	0.77
(1,292)	1:21:A:ARG:HA	1:22:A:PRO:HD3	2	0.76	0.22	0.76
(1,322)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	2	0.6	0.04	0.6
(1,245)	1:7:A:LEU:HB2	1:8:A:TYR:H	2	0.52	0.18	0.52
(1,127)	1:14:A:GLN:H	1:14:A:GLN:HA	2	0.52	0.0	0.52
(1,108)	1:6:A:ARG:H	1:6:A:ARG:HB2	2	0.48	0.04	0.48
(1,227)	1:13:A:LYS:HA	1:14:A:GLN:H	2	0.44	0.2	0.44
(1,331)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	2	0.44	0.32	0.44
(1,331)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	2	0.44	0.32	0.44
(1,331)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	2	0.44	0.32	0.44
(1,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	2	0.38	0.19	0.38
(1,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	2	0.36	0.01	0.36
(1,280)	1:4:A:ALA:H	1:5:A:VAL:H	2	0.34	0.16	0.34
(2,168)	1:7:A:LEU:H	1:7:A:LEU:HD11	2	0.32	0.16	0.32
(2,168)	1:7:A:LEU:H	1:7:A:LEU:HD12	2	0.32	0.16	0.32
(2,168)	1:7:A:LEU:H	1:7:A:LEU:HD13	2	0.32	0.16	0.32
(3,161)	1:7:A:LEU:H	1:7:A:LEU:HD11	2	0.32	0.16	0.32
(3,161)	1:7:A:LEU:H	1:7:A:LEU:HD12	2	0.32	0.16	0.32
(3,161)	1:7:A:LEU:H	1:7:A:LEU:HD13	2	0.32	0.16	0.32
(1,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	2	0.28	0.06	0.28
(1,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	2	0.28	0.06	0.28
(1,330)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	2	0.27	0.06	0.27
(1,330)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	2	0.27	0.06	0.27
(1,330)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	2	0.27	0.06	0.27
(2,299)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	2	0.24	0.12	0.24
(3,286)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	2	0.24	0.12	0.24
(1,237)	1:3:A:GLU:H	1:3:A:GLU:HB3	2	0.22	0.08	0.22
(2,245)	1:7:A:LEU:HB2	1:8:A:TYR:H	2	0.17	0.01	0.17
(4,11)	1:7:A:LEU:HB2	1:8:A:TYR:H	2	0.17	0.01	0.17
(2,289)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	2	0.16	0.06	0.16
(2,289)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	2	0.16	0.06	0.16

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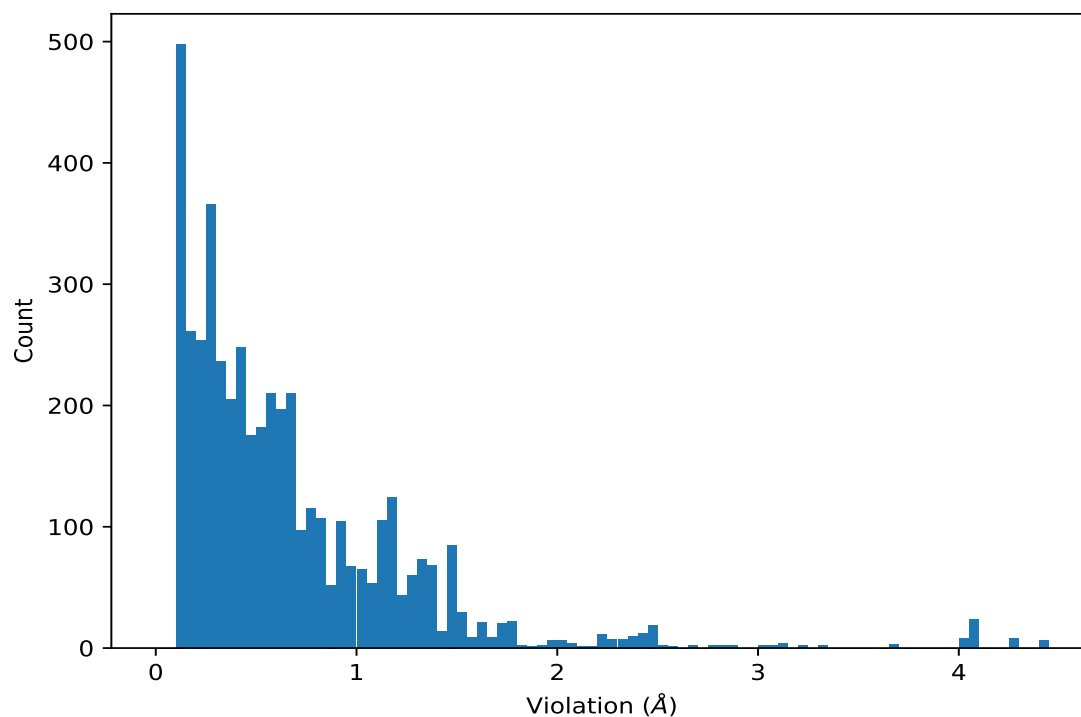
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,276)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	2	0.16	0.06	0.16
(3,276)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	2	0.16	0.06	0.16
(2,238)	1:3:A:GLU:H	1:3:A:GLU:HB2	2	0.16	0.01	0.16
(3,229)	1:3:A:GLU:H	1:3:A:GLU:HB2	2	0.16	0.01	0.16
(1,142)	1:12:A:LEU:H	1:13:A:LYS:H	2	0.15	0.04	0.15
(1,300)	1:23:A:PRO:HA	1:24:A:PRO:HD3	2	0.14	0.02	0.14
(2,300)	1:23:A:PRO:HA	1:24:A:PRO:HD3	2	0.13	0.02	0.13
(3,287)	1:23:A:PRO:HA	1:24:A:PRO:HD3	2	0.13	0.02	0.13

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)
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	4	4.43
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	4	4.43
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	4	4.43
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	4	4.43
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	4	4.43
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	4	4.43
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	3	4.27
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	3	4.27
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	3	4.27
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	3	4.27
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	10	4.26
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	10	4.26
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	10	4.26
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	10	4.26
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	5	4.09
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	5	4.09
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	5	4.09
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	5	4.09
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	2	4.08
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	2	4.08
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	2	4.08
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	2	4.08
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	8	4.08
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	8	4.08
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	8	4.08
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	8	4.08
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	4	4.07
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	4	4.07
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	4	4.07
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	4	4.07
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	7	4.07
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	7	4.07
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	7	4.07
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	7	4.07
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	9	4.06
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	9	4.06
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	9	4.06
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	9	4.06
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	1	4.04
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	1	4.04
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	1	4.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	1	4.04
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	6	4.03
(1,214)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	6	4.03
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	6	4.03
(1,214)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	6	4.03
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	4	3.67
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	4	3.67
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	4	3.67
(4,9)	1:5:A:VAL:H	1:7:A:LEU:HA	2	3.32
(2,234)	1:5:A:VAL:H	1:7:A:LEU:HA	2	3.32
(4,9)	1:5:A:VAL:H	1:7:A:LEU:HA	7	3.23
(2,234)	1:5:A:VAL:H	1:7:A:LEU:HA	7	3.23
(4,9)	1:5:A:VAL:H	1:7:A:LEU:HA	4	3.14
(2,234)	1:5:A:VAL:H	1:7:A:LEU:HA	4	3.14
(4,9)	1:5:A:VAL:H	1:7:A:LEU:HA	5	3.11
(2,234)	1:5:A:VAL:H	1:7:A:LEU:HA	5	3.11
(4,9)	1:5:A:VAL:H	1:7:A:LEU:HA	9	3.09
(2,234)	1:5:A:VAL:H	1:7:A:LEU:HA	9	3.09
(4,9)	1:5:A:VAL:H	1:7:A:LEU:HA	6	3.03
(2,234)	1:5:A:VAL:H	1:7:A:LEU:HA	6	3.03
(3,299)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	4	2.9
(2,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	4	2.9
(3,299)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	10	2.83
(2,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	10	2.83
(4,9)	1:5:A:VAL:H	1:7:A:LEU:HA	8	2.78
(2,234)	1:5:A:VAL:H	1:7:A:LEU:HA	8	2.78
(4,9)	1:5:A:VAL:H	1:7:A:LEU:HA	3	2.69
(2,234)	1:5:A:VAL:H	1:7:A:LEU:HA	3	2.69
(1,234)	1:5:A:VAL:H	1:7:A:LEU:HA	2	2.57
(4,9)	1:5:A:VAL:H	1:7:A:LEU:HA	10	2.5
(2,234)	1:5:A:VAL:H	1:7:A:LEU:HA	10	2.5
(1,234)	1:5:A:VAL:H	1:7:A:LEU:HA	7	2.49
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	2	2.47
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	2	2.47
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	2	2.47
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	5	2.47
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	5	2.47
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	5	2.47
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	2	2.47
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	2	2.47
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	2	2.47
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	5	2.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	5	2.47
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	5	2.47
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	8	2.45
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	8	2.45
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	8	2.45
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	8	2.45
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	8	2.45
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	8	2.45
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	7	2.42
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	7	2.42
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	7	2.42
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	7	2.42
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	7	2.42
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	7	2.42
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	10	2.41
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	10	2.41
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	10	2.41
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	10	2.41
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	10	2.41
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	10	2.41
(1,234)	1:5:A:VAL:H	1:7:A:LEU:HA	4	2.4
(1,234)	1:5:A:VAL:H	1:7:A:LEU:HA	5	2.37
(4,9)	1:5:A:VAL:H	1:7:A:LEU:HA	1	2.36
(2,234)	1:5:A:VAL:H	1:7:A:LEU:HA	1	2.36
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	6	2.35
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	6	2.35
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	6	2.35
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	6	2.35
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	6	2.35
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	6	2.35
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	9	2.34
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	9	2.34
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	9	2.34
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	9	2.34
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	9	2.34
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	9	2.34
(1,234)	1:5:A:VAL:H	1:7:A:LEU:HA	9	2.34
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	1	2.3
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	1	2.3
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	1	2.3
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	1	2.3
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	1	2.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	1	2.3
(1,234)	1:5:A:VAL:H	1:7:A:LEU:HA	6	2.29
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD2	9	2.24
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD3	9	2.24
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	3	2.21
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	3	2.21
(4,12)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	3	2.21
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	3	2.21
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	3	2.21
(2,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	3	2.21
(1,120)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	2	2.21
(3,306)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	2	2.2
(2,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	2	2.2
(1,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	4	2.15
(1,120)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	3	2.14
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD2	3	2.09
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD3	3	2.09
(1,120)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	10	2.09
(1,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	10	2.08
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD2	1	2.05
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD3	1	2.05
(1,106)	1:6:A:ARG:HA	1:6:A:ARG:HG2	4	2.04
(1,234)	1:5:A:VAL:H	1:7:A:LEU:HA	8	2.03
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD2	7	2.02
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD3	7	2.02
(1,120)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	7	1.99
(1,106)	1:6:A:ARG:HA	1:6:A:ARG:HG2	2	1.98
(1,120)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	8	1.97
(1,120)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	1	1.96
(1,120)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	6	1.96
(1,120)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	9	1.96
(1,234)	1:5:A:VAL:H	1:7:A:LEU:HA	3	1.95
(1,120)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	5	1.95
(1,117)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	3	1.87
(3,299)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	3	1.81
(2,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	3	1.81
(1,114)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	6	1.79
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	2	1.76
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	2	1.76
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	2	1.76
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	2	1.76
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	2	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	2	1.76
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	2	1.76
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	2	1.76
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	2	1.76
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	2	1.76
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	2	1.76
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	2	1.76
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	2	1.76
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	2	1.76
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	2	1.76
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	2	1.76
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	2	1.76
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	2	1.76
(1,234)	1:5:A:VAL:H	1:7:A:LEU:HA	10	1.76
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD2	8	1.75
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD3	8	1.75
(4,14)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	2	1.74
(3,312)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	2	1.74
(3,312)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	2	1.74
(3,312)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	2	1.74
(2,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	2	1.74
(2,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	2	1.74
(2,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	2	1.74
(2,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	2	1.74
(4,14)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	3	1.71
(4,14)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	7	1.71
(3,306)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	7	1.71
(2,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	7	1.71
(2,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	3	1.71
(2,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	7	1.71
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	2	1.71
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	2	1.71
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	2	1.71
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	5	1.71
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	5	1.71
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	5	1.71
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	8	1.69
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	8	1.69
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	8	1.69
(4,14)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	1	1.67
(2,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	1	1.67
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	7	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	7	1.66
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	7	1.66
(1,110)	1:6:A:ARG:H	1:6:A:ARG:HG3	9	1.66
(4,14)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	6	1.65
(2,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	6	1.65
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	10	1.65
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	10	1.65
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	10	1.65
(4,14)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	10	1.64
(2,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	10	1.64
(1,117)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	10	1.64
(4,14)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	9	1.62
(2,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	9	1.62
(1,234)	1:5:A:VAL:H	1:7:A:LEU:HA	1	1.62
(1,196)	1:12:A:LEU:HA	1:12:A:LEU:HD21	4	1.62
(1,196)	1:12:A:LEU:HA	1:12:A:LEU:HD22	4	1.62
(1,196)	1:12:A:LEU:HA	1:12:A:LEU:HD23	4	1.62
(1,114)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	4	1.62
(4,14)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	5	1.6
(2,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	5	1.6
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	6	1.6
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	6	1.6
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	6	1.6
(1,110)	1:6:A:ARG:H	1:6:A:ARG:HG3	1	1.6
(3,299)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	6	1.59
(2,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	6	1.59
(1,267)	1:18:A:SER:H	1:18:A:SER:HB2	3	1.59
(1,267)	1:18:A:SER:H	1:18:A:SER:HB3	3	1.59
(3,296)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	1.58
(2,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	1.58
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	9	1.58
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	9	1.58
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	9	1.58
(3,296)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	1.54
(2,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	1.54
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	1	1.54
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	1	1.54
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	1	1.54
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	5	1.53
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	5	1.53
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	5	1.53
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	5	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	5	1.53
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	5	1.53
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	5	1.53
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	5	1.53
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	5	1.53
(3,296)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	1.53
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	5	1.53
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	5	1.53
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	5	1.53
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	5	1.53
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	5	1.53
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	5	1.53
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	5	1.53
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	5	1.53
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	5	1.53
(2,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	1.53
(3,296)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	1.52
(2,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	1.52
(3,306)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	4	1.5
(2,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	4	1.5
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	2	1.49
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	2	1.49
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	2	1.49
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	2	1.49
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	2	1.49
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	2	1.49
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	2	1.49
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	2	1.49
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	2	1.49
(3,296)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	1.49
(3,296)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	1.49
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	2	1.49
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	2	1.49
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	2	1.49
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	2	1.49
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	2	1.49
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	2	1.49
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	2	1.49
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	2	1.49
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	2	1.49
(2,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	1.49
(2,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,322)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	2	1.48
(3,322)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	2	1.48
(3,322)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	2	1.48
(2,337)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	2	1.48
(2,337)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	2	1.48
(2,337)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	2	1.48
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	5	1.47
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	5	1.47
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	5	1.47
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	5	1.47
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	5	1.47
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	5	1.47
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	5	1.47
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	5	1.47
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	5	1.47
(3,299)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	2	1.47
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	5	1.47
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	5	1.47
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	5	1.47
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	5	1.47
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	5	1.47
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	5	1.47
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	5	1.47
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	5	1.47
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	5	1.47
(2,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	2	1.47
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	3	1.46
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	3	1.46
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	3	1.46
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	3	1.46
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	3	1.46
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	3	1.46
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	3	1.46
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	3	1.46
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	3	1.46
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	8	1.46
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	8	1.46
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	8	1.46
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	8	1.46
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	8	1.46
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	8	1.46
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	8	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	8	1.46
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	8	1.46
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	3	1.46
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	3	1.46
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	3	1.46
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	3	1.46
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	3	1.46
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	3	1.46
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	3	1.46
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	3	1.46
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	3	1.46
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	8	1.46
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	8	1.46
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	8	1.46
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	8	1.46
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	8	1.46
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	8	1.46
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	8	1.46
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	8	1.46
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	8	1.46
(1,120)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	4	1.46
(3,296)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	1.45
(2,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	1.45
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD11	3	1.45
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD12	3	1.45
(1,254)	1:11:A:TRP:HD1	1:12:A:LEU:HD13	3	1.45
(1,72)	1:23:A:PRO:HA	1:23:A:PRO:HG3	6	1.45
(1,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	2	1.44
(3,306)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	8	1.43
(2,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	8	1.43
(1,91)	1:24:A:PRO:HA	1:24:A:PRO:HG3	5	1.43
(1,91)	1:24:A:PRO:HA	1:24:A:PRO:HG3	6	1.42
(1,18)	1:19:A:SER:H	1:19:A:SER:HA	5	1.41
(1,18)	1:19:A:SER:H	1:19:A:SER:HA	8	1.41
(1,18)	1:19:A:SER:H	1:19:A:SER:HA	10	1.41
(3,312)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	7	1.4
(3,312)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	7	1.4
(3,312)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	7	1.4
(2,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	7	1.4
(2,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	7	1.4
(2,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	7	1.4
(3,296)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	7	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	7	1.39
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG2	4	1.39
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG3	4	1.39
(1,110)	1:6:A:ARG:H	1:6:A:ARG:HG3	5	1.39
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	4	1.38
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	4	1.38
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	4	1.38
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	4	1.38
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	4	1.38
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	4	1.38
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	4	1.38
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	4	1.38
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	4	1.38
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	4	1.38
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	4	1.38
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	4	1.38
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	4	1.38
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	4	1.38
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	4	1.38
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	4	1.38
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	4	1.38
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	4	1.38
(4,2)	1:22:A:PRO:HA	1:22:A:PRO:HD2	5	1.37
(3,312)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	5	1.37
(3,312)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	5	1.37
(3,312)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	5	1.37
(2,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	5	1.37
(2,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	5	1.37
(2,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	5	1.37
(2,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	5	1.37
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	10	1.36
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	10	1.36
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	10	1.36
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	10	1.36
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	10	1.36
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	10	1.36
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	10	1.36
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	10	1.36
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	10	1.36
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	10	1.36
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	10	1.36
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	10	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	10	1.36
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	10	1.36
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	10	1.36
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	10	1.36
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	10	1.36
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	10	1.36
(1,268)	1:18:A:SER:H	1:18:A:SER:HA	3	1.36
(1,268)	1:18:A:SER:H	1:18:A:SER:HA	4	1.36
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG2	5	1.36
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG3	5	1.36
(1,21)	1:15:A:GLY:H	1:15:A:GLY:HA2	6	1.36
(1,21)	1:15:A:GLY:H	1:15:A:GLY:HA2	7	1.36
(1,180)	1:9:A:ILE:HB	1:9:A:ILE:HG13	5	1.35
(1,180)	1:9:A:ILE:HB	1:9:A:ILE:HG13	9	1.35
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD21	2	1.35
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD22	2	1.35
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD23	2	1.35
(1,91)	1:24:A:PRO:HA	1:24:A:PRO:HG3	9	1.35
(1,21)	1:15:A:GLY:H	1:15:A:GLY:HA2	3	1.35
(3,299)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	8	1.34
(2,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	8	1.34
(1,268)	1:18:A:SER:H	1:18:A:SER:HA	7	1.34
(1,268)	1:18:A:SER:H	1:18:A:SER:HA	9	1.34
(1,21)	1:15:A:GLY:H	1:15:A:GLY:HA2	4	1.34
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	8	1.33
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	8	1.33
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	8	1.33
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	8	1.33
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	8	1.33
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	8	1.33
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	8	1.33
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	8	1.33
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	8	1.33
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	8	1.33
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	8	1.33
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	8	1.33
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	8	1.33
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	8	1.33
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	8	1.33
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	8	1.33
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	8	1.33
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	8	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,268)	1:18:A:SER:H	1:18:A:SER:HA	1	1.33
(1,268)	1:18:A:SER:H	1:18:A:SER:HA	5	1.33
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG2	6	1.33
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG3	6	1.33
(1,180)	1:9:A:ILE:HB	1:9:A:ILE:HG13	2	1.33
(1,180)	1:9:A:ILE:HB	1:9:A:ILE:HG13	7	1.33
(1,21)	1:15:A:GLY:H	1:15:A:GLY:HA2	1	1.33
(1,21)	1:15:A:GLY:H	1:15:A:GLY:HA2	2	1.33
(1,268)	1:18:A:SER:H	1:18:A:SER:HA	2	1.32
(1,268)	1:18:A:SER:H	1:18:A:SER:HA	6	1.32
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG2	2	1.32
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG3	2	1.32
(1,21)	1:15:A:GLY:H	1:15:A:GLY:HA2	5	1.32
(1,21)	1:15:A:GLY:H	1:15:A:GLY:HA2	8	1.32
(4,15)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	7	1.31
(3,306)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	1	1.31
(3,306)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	3	1.31
(2,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	1	1.31
(2,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	3	1.31
(2,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	7	1.31
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG2	8	1.31
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG3	8	1.31
(1,158)	1:7:A:LEU:HB3	1:7:A:LEU:HG	3	1.31
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	7	1.3
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	7	1.3
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	7	1.3
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	7	1.3
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	7	1.3
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	7	1.3
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	7	1.3
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	7	1.3
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	7	1.3
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	7	1.3
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	7	1.3
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	7	1.3
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	7	1.3
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	7	1.3
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	7	1.3
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	7	1.3
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	7	1.3
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	7	1.3
(1,284)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	6	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,268)	1:18:A:SER:H	1:18:A:SER:HA	8	1.3
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG2	10	1.3
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG3	10	1.3
(1,158)	1:7:A:LEU:HB3	1:7:A:LEU:HG	1	1.3
(1,158)	1:7:A:LEU:HB3	1:7:A:LEU:HG	10	1.3
(1,106)	1:6:A:ARG:HA	1:6:A:ARG:HG2	6	1.3
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	5	1.3
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	5	1.3
(3,299)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	7	1.29
(2,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	7	1.29
(1,288)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	5	1.29
(1,288)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	5	1.29
(1,267)	1:18:A:SER:H	1:18:A:SER:HB2	1	1.29
(1,267)	1:18:A:SER:H	1:18:A:SER:HB3	1	1.29
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG2	7	1.29
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG3	7	1.29
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	8	1.29
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	8	1.29
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG2	1	1.28
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG3	1	1.28
(1,199)	1:12:A:LEU:HA	1:12:A:LEU:HG	2	1.28
(1,91)	1:24:A:PRO:HA	1:24:A:PRO:HG3	1	1.28
(4,2)	1:22:A:PRO:HA	1:22:A:PRO:HD2	3	1.27
(4,2)	1:22:A:PRO:HA	1:22:A:PRO:HD2	4	1.27
(4,2)	1:22:A:PRO:HA	1:22:A:PRO:HD2	9	1.27
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	4	1.27
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	4	1.27
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	4	1.27
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	4	1.27
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	4	1.27
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	4	1.27
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	4	1.27
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	4	1.27
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	4	1.27
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	4	1.27
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	4	1.27
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	4	1.27
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	4	1.27
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	4	1.27
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	4	1.27
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	4	1.27
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	4	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	4	1.27
(2,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	3	1.27
(2,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	4	1.27
(2,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	9	1.27
(1,171)	1:9:A:ILE:HA	1:9:A:ILE:HG12	7	1.27
(1,91)	1:24:A:PRO:HA	1:24:A:PRO:HG3	3	1.27
(1,91)	1:24:A:PRO:HA	1:24:A:PRO:HG3	10	1.27
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	6	1.27
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	6	1.27
(4,2)	1:22:A:PRO:HA	1:22:A:PRO:HD2	1	1.26
(4,2)	1:22:A:PRO:HA	1:22:A:PRO:HD2	8	1.26
(3,296)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	1.26
(2,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	1.26
(2,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	1	1.26
(2,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	8	1.26
(1,199)	1:12:A:LEU:HA	1:12:A:LEU:HG	8	1.26
(4,2)	1:22:A:PRO:HA	1:22:A:PRO:HD2	2	1.25
(2,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	2	1.25
(1,267)	1:18:A:SER:H	1:18:A:SER:HB2	2	1.25
(1,267)	1:18:A:SER:H	1:18:A:SER:HB3	2	1.25
(1,267)	1:18:A:SER:H	1:18:A:SER:HB2	9	1.25
(1,267)	1:18:A:SER:H	1:18:A:SER:HB3	9	1.25
(1,199)	1:12:A:LEU:HA	1:12:A:LEU:HG	3	1.25
(1,199)	1:12:A:LEU:HA	1:12:A:LEU:HG	5	1.25
(1,91)	1:24:A:PRO:HA	1:24:A:PRO:HG3	2	1.25
(1,73)	1:23:A:PRO:HA	1:23:A:PRO:HG2	4	1.25
(4,2)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	1.24
(2,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	1.24
(1,267)	1:18:A:SER:H	1:18:A:SER:HB2	7	1.24
(1,267)	1:18:A:SER:H	1:18:A:SER:HB3	7	1.24
(1,199)	1:12:A:LEU:HA	1:12:A:LEU:HG	6	1.24
(1,199)	1:12:A:LEU:HA	1:12:A:LEU:HG	7	1.24
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	7	1.23
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	7	1.23
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	7	1.23
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	7	1.23
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	7	1.23
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	7	1.23
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	7	1.23
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	7	1.23
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	7	1.23
(3,306)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	10	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	7	1.23
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	7	1.23
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	7	1.23
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	7	1.23
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	7	1.23
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	7	1.23
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	7	1.23
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	7	1.23
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	7	1.23
(2,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	10	1.23
(1,267)	1:18:A:SER:H	1:18:A:SER:HB2	4	1.23
(1,267)	1:18:A:SER:H	1:18:A:SER:HB3	4	1.23
(1,171)	1:9:A:ILE:HA	1:9:A:ILE:HG12	9	1.23
(1,158)	1:7:A:LEU:HB3	1:7:A:LEU:HG	8	1.23
(1,117)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	1	1.23
(4,2)	1:22:A:PRO:HA	1:22:A:PRO:HD2	7	1.22
(2,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	7	1.22
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	3	1.22
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	3	1.22
(1,199)	1:12:A:LEU:HA	1:12:A:LEU:HG	9	1.21
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD21	6	1.21
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD22	6	1.21
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD23	6	1.21
(1,73)	1:23:A:PRO:HA	1:23:A:PRO:HG2	1	1.21
(1,73)	1:23:A:PRO:HA	1:23:A:PRO:HG2	3	1.21
(1,73)	1:23:A:PRO:HA	1:23:A:PRO:HG2	5	1.21
(1,73)	1:23:A:PRO:HA	1:23:A:PRO:HG2	7	1.21
(1,268)	1:18:A:SER:H	1:18:A:SER:HA	10	1.2
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	4	1.2
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	4	1.2
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	4	1.2
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	4	1.2
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	9	1.2
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	9	1.2
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	9	1.2
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	9	1.2
(1,199)	1:12:A:LEU:HA	1:12:A:LEU:HG	1	1.2
(1,180)	1:9:A:ILE:HB	1:9:A:ILE:HG13	3	1.2
(1,180)	1:9:A:ILE:HB	1:9:A:ILE:HG13	10	1.2
(1,73)	1:23:A:PRO:HA	1:23:A:PRO:HG2	2	1.2
(1,73)	1:23:A:PRO:HA	1:23:A:PRO:HG2	9	1.2
(1,73)	1:23:A:PRO:HA	1:23:A:PRO:HG2	10	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,14)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	8	1.19
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	1.19
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	1.19
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	1.19
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	1.19
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	1.19
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	1.19
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	1.19
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	1.19
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	1.19
(2,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	8	1.19
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	1.19
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	1.19
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	1.19
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	1.19
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	1.19
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	1.19
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	1.19
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	1.19
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	1.19
(1,334)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	10	1.19
(1,334)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	10	1.19
(1,334)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	10	1.19
(1,334)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	10	1.19
(1,334)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	10	1.19
(1,334)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	10	1.19
(1,252)	1:5:A:VAL:HG11	1:6:A:ARG:H	2	1.19
(1,252)	1:5:A:VAL:HG12	1:6:A:ARG:H	2	1.19
(1,252)	1:5:A:VAL:HG13	1:6:A:ARG:H	2	1.19
(1,252)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	1.19
(1,252)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	1.19
(1,252)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	1	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	1	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	1	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	1	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	2	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	2	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	2	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	2	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	5	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	5	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	5	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	5	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	6	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	6	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	6	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	6	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	7	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	7	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	7	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	7	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	8	1.19
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	8	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	8	1.19
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	8	1.19
(1,180)	1:9:A:ILE:HB	1:9:A:ILE:HG13	1	1.19
(1,180)	1:9:A:ILE:HB	1:9:A:ILE:HG13	8	1.19
(1,73)	1:23:A:PRO:HA	1:23:A:PRO:HG2	8	1.19
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	1.18
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	1.18
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	1.18
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	1.18
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	1.18
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	1.18
(1,199)	1:12:A:LEU:HA	1:12:A:LEU:HG	10	1.18
(1,180)	1:9:A:ILE:HB	1:9:A:ILE:HG13	4	1.18
(1,180)	1:9:A:ILE:HB	1:9:A:ILE:HG13	6	1.18
(1,158)	1:7:A:LEU:HB3	1:7:A:LEU:HG	4	1.18
(1,117)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	5	1.18
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	1.17
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	1.17
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	1.17
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	6	1.17
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	6	1.17
(3,310)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	6	1.17
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	6	1.17
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	6	1.17
(3,310)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	6	1.17
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	6	1.17
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	6	1.17
(3,310)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	6	1.17
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	6	1.17
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	6	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,325)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	6	1.17
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	6	1.17
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	6	1.17
(2,325)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	6	1.17
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	6	1.17
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	6	1.17
(2,325)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	6	1.17
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	1.17
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	1.17
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	1.17
(1,337)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	1	1.17
(1,337)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	1	1.17
(1,337)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	1	1.17
(1,313)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	5	1.17
(1,285)	1:3:A:GLU:HB2	1:4:A:ALA:H	5	1.16
(1,252)	1:5:A:VAL:HG11	1:6:A:ARG:H	4	1.16
(1,252)	1:5:A:VAL:HG12	1:6:A:ARG:H	4	1.16
(1,252)	1:5:A:VAL:HG13	1:6:A:ARG:H	4	1.16
(1,252)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	1.16
(1,252)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	1.16
(1,252)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	1.16
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG2	3	1.16
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG3	3	1.16
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	4	1.16
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	4	1.16
(1,337)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	10	1.15
(1,337)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	10	1.15
(1,337)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	10	1.15
(1,252)	1:5:A:VAL:HG11	1:6:A:ARG:H	8	1.15
(1,252)	1:5:A:VAL:HG12	1:6:A:ARG:H	8	1.15
(1,252)	1:5:A:VAL:HG13	1:6:A:ARG:H	8	1.15
(1,252)	1:5:A:VAL:HG21	1:6:A:ARG:H	8	1.15
(1,252)	1:5:A:VAL:HG22	1:6:A:ARG:H	8	1.15
(1,252)	1:5:A:VAL:HG23	1:6:A:ARG:H	8	1.15
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	9	1.14
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	9	1.14
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	9	1.14
(1,252)	1:5:A:VAL:HG11	1:6:A:ARG:H	5	1.14
(1,252)	1:5:A:VAL:HG12	1:6:A:ARG:H	5	1.14
(1,252)	1:5:A:VAL:HG13	1:6:A:ARG:H	5	1.14
(1,252)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	1.14
(1,252)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	1.14
(1,171)	1:9:A:ILE:HA	1:9:A:ILE:HG12	2	1.14
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	7	1.14
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	7	1.14
(4,2)	1:22:A:PRO:HA	1:22:A:PRO:HD2	6	1.13
(2,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	6	1.13
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	3	1.13
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	3	1.13
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	3	1.13
(1,171)	1:9:A:ILE:HA	1:9:A:ILE:HG12	5	1.13
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	1	1.13
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	1	1.13
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	1	1.13
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	1	1.13
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	4	1.13
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	4	1.13
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	4	1.13
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	4	1.13
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	9	1.13
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	9	1.13
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	9	1.13
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	9	1.13
(4,4)	1:24:A:PRO:HA	1:24:A:PRO:HD3	8	1.12
(2,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	8	1.12
(1,313)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	2	1.12
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	1.12
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	1.12
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	1.12
(1,239)	1:3:A:GLU:HB3	1:4:A:ALA:H	7	1.12
(1,158)	1:7:A:LEU:HB3	1:7:A:LEU:HG	5	1.12
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	1	1.12
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	1	1.12
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	2	1.12
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	2	1.12
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	3	1.12
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	3	1.12
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	2	1.12
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	2	1.12
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	2	1.12
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	2	1.12
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	10	1.12
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	10	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	10	1.12
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	10	1.12
(1,337)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	3	1.11
(1,337)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	3	1.11
(1,337)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	3	1.11
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	1	1.11
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	1	1.11
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	1	1.11
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	1.11
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	1.11
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	1.11
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	6	1.11
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	6	1.11
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	6	1.11
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	3	1.11
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	3	1.11
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	3	1.11
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	3	1.11
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	1.11
(1,209)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	10	1.11
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	10	1.11
(1,209)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	10	1.11
(1,117)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	9	1.11
(1,73)	1:23:A:PRO:HA	1:23:A:PRO:HG2	6	1.11
(4,4)	1:24:A:PRO:HA	1:24:A:PRO:HD3	4	1.1
(2,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	4	1.1
(1,313)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	1	1.1
(1,285)	1:3:A:GLU:HB2	1:4:A:ALA:H	9	1.1
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	5	1.1
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	5	1.1
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	5	1.1
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	7	1.1
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	7	1.1
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	7	1.1
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	8	1.1
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	8	1.1
(1,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	8	1.1
(1,252)	1:5:A:VAL:HG11	1:6:A:ARG:H	10	1.1
(1,252)	1:5:A:VAL:HG12	1:6:A:ARG:H	10	1.1
(1,252)	1:5:A:VAL:HG13	1:6:A:ARG:H	10	1.1
(1,252)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	1.1
(1,252)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	1.1
(1,223)	1:15:A:GLY:H	1:16:A:GLY:H	9	1.1
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	9	1.1
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	9	1.1
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	5	1.09
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	5	1.09
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	10	1.09
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	10	1.09
(3,247)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	7	1.08
(3,247)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	7	1.08
(2,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	7	1.08
(2,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	7	1.08
(1,324)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	7	1.08
(1,324)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	7	1.08
(1,324)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	7	1.08
(1,324)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	7	1.08
(1,324)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	7	1.08
(1,324)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	7	1.08
(1,313)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	10	1.08
(1,288)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	8	1.08
(1,288)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	8	1.08
(1,270)	1:19:A:SER:H	1:19:A:SER:HB3	2	1.08
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	1	1.08
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	1	1.08
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	1	1.08
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	1	1.08
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	7	1.08
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	7	1.08
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	7	1.08
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	7	1.08
(1,80)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	4	1.08
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	8	1.07
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	8	1.07
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	8	1.07
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	8	1.07
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	9	1.07
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	9	1.07
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	9	1.07
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	9	1.07
(1,117)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	8	1.07
(1,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	3	1.06
(1,313)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	3	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	2	1.06
(1,288)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	2	1.06
(1,267)	1:18:A:SER:H	1:18:A:SER:HB2	10	1.06
(1,267)	1:18:A:SER:H	1:18:A:SER:HB3	10	1.06
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	3	1.06
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	3	1.06
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	3	1.06
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	3	1.06
(1,80)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	5	1.06
(1,252)	1:5:A:VAL:HG11	1:6:A:ARG:H	7	1.05
(1,252)	1:5:A:VAL:HG12	1:6:A:ARG:H	7	1.05
(1,252)	1:5:A:VAL:HG13	1:6:A:ARG:H	7	1.05
(1,252)	1:5:A:VAL:HG21	1:6:A:ARG:H	7	1.05
(1,252)	1:5:A:VAL:HG22	1:6:A:ARG:H	7	1.05
(1,252)	1:5:A:VAL:HG23	1:6:A:ARG:H	7	1.05
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD11	5	1.04
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD12	5	1.04
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD13	5	1.04
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	8	1.04
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	8	1.04
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	3	1.04
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	3	1.04
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	3	1.04
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	3	1.04
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	5	1.04
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	5	1.04
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	5	1.04
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	5	1.04
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	8	1.04
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	8	1.04
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	8	1.04
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	8	1.04
(1,329)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	6	1.03
(1,329)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	6	1.03
(1,329)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	6	1.03
(1,324)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	9	1.03
(1,324)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	9	1.03
(1,324)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	9	1.03
(1,324)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	9	1.03
(1,324)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	9	1.03
(1,324)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	9	1.03
(1,247)	1:21:A:ARG:H	1:21:A:ARG:HG2	4	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD21	7	1.03
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD22	7	1.03
(1,169)	1:7:A:LEU:H	1:7:A:LEU:HD23	7	1.03
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	6	1.03
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	6	1.03
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	6	1.03
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	6	1.03
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	7	1.03
(1,41)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	7	1.03
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	7	1.03
(1,41)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	7	1.03
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	2	1.02
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	2	1.02
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	2	1.02
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	2	1.02
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	2	1.02
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	2	1.02
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	2	1.02
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	2	1.02
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	2	1.02
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	2	1.02
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	2	1.02
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	2	1.02
(1,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	2	1.02
(1,139)	1:5:A:VAL:H	1:6:A:ARG:H	1	1.02
(1,291)	1:21:A:ARG:HA	1:22:A:PRO:HD2	10	1.01
(1,270)	1:19:A:SER:H	1:19:A:SER:HB3	3	1.01
(1,291)	1:21:A:ARG:HA	1:22:A:PRO:HD2	8	1.0
(1,270)	1:19:A:SER:H	1:19:A:SER:HB3	9	1.0
(1,252)	1:5:A:VAL:HG11	1:6:A:ARG:H	3	1.0
(1,252)	1:5:A:VAL:HG12	1:6:A:ARG:H	3	1.0
(1,252)	1:5:A:VAL:HG13	1:6:A:ARG:H	3	1.0
(1,252)	1:5:A:VAL:HG21	1:6:A:ARG:H	3	1.0
(1,252)	1:5:A:VAL:HG22	1:6:A:ARG:H	3	1.0
(1,252)	1:5:A:VAL:HG23	1:6:A:ARG:H	3	1.0
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG2	9	1.0
(1,212)	1:13:A:LYS:HA	1:13:A:LYS:HG3	9	1.0
(1,139)	1:5:A:VAL:H	1:6:A:ARG:H	3	1.0
(1,320)	1:16:A:GLY:HA2	1:21:A:ARG:HB2	2	0.99
(1,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	3	0.99
(1,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	7	0.99
(1,288)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	10	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	10	0.99
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD11	3	0.99
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD12	3	0.99
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD13	3	0.99
(1,329)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	7	0.98
(1,329)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	7	0.98
(1,329)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	7	0.98
(1,292)	1:21:A:ARG:HA	1:22:A:PRO:HD3	6	0.98
(1,291)	1:21:A:ARG:HA	1:22:A:PRO:HD2	2	0.98
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	1	0.98
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	1	0.98
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	1	0.98
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	1	0.98
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	1	0.98
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	1	0.98
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	1	0.98
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	1	0.98
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	1	0.98
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	1	0.98
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	1	0.98
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	1	0.98
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	2	0.98
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	2	0.98
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	2	0.98
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	2	0.98
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	4	0.98
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	4	0.98
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	4	0.98
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	4	0.98
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	5	0.98
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	5	0.98
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	5	0.98
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	5	0.98
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	6	0.98
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	6	0.98
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	6	0.98
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	6	0.98
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	0.98
(1,216)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	0.98
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	10	0.98
(1,216)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	10	0.98
(3,247)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	3	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,247)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	3	0.97
(2,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	3	0.97
(2,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	3	0.97
(1,332)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	2	0.97
(1,332)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	2	0.97
(1,332)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	2	0.97
(1,309)	1:9:A:ILE:HA	1:12:A:LEU:HB2	9	0.97
(1,329)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	8	0.96
(1,329)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	8	0.96
(1,329)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	8	0.96
(1,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	7	0.96
(1,315)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	1	0.96
(1,284)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	7	0.96
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD11	10	0.96
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD12	10	0.96
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD13	10	0.96
(1,118)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	4	0.96
(1,117)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	7	0.96
(1,89)	1:24:A:PRO:HA	1:24:A:PRO:HB3	7	0.96
(1,61)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	3	0.96
(1,61)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	4	0.96
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.95
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.95
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.95
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.95
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.95
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.95
(1,329)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	4	0.95
(1,329)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	4	0.95
(1,329)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	4	0.95
(1,309)	1:9:A:ILE:HA	1:12:A:LEU:HB2	1	0.95
(1,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	1	0.95
(1,291)	1:21:A:ARG:HA	1:22:A:PRO:HD2	1	0.95
(1,273)	1:13:A:LYS:H	1:14:A:GLN:H	2	0.95
(1,118)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	6	0.95
(1,89)	1:24:A:PRO:HA	1:24:A:PRO:HB3	4	0.95
(1,80)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	6	0.95
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	10	0.94
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	10	0.94
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	10	0.94
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	10	0.94
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	10	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	10	0.94
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	10	0.94
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	10	0.94
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	10	0.94
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	10	0.94
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	10	0.94
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	10	0.94
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	10	0.94
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	10	0.94
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	10	0.94
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	10	0.94
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	10	0.94
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	10	0.94
(1,315)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	7	0.94
(1,291)	1:21:A:ARG:HA	1:22:A:PRO:HD2	7	0.94
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD11	1	0.94
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD12	1	0.94
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD13	1	0.94
(1,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	6	0.93
(1,260)	1:4:A:ALA:HB1	1:5:A:VAL:H	4	0.93
(1,260)	1:4:A:ALA:HB2	1:5:A:VAL:H	4	0.93
(1,260)	1:4:A:ALA:HB3	1:5:A:VAL:H	4	0.93
(1,61)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	9	0.93
(4,15)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	10	0.92
(3,320)	1:7:A:LEU:HD11	1:8:A:TYR:HB2	2	0.92
(3,320)	1:7:A:LEU:HD12	1:8:A:TYR:HB2	2	0.92
(3,320)	1:7:A:LEU:HD13	1:8:A:TYR:HB2	2	0.92
(2,335)	1:7:A:LEU:HD11	1:8:A:TYR:HB2	2	0.92
(2,335)	1:7:A:LEU:HD12	1:8:A:TYR:HB2	2	0.92
(2,335)	1:7:A:LEU:HD13	1:8:A:TYR:HB2	2	0.92
(2,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	10	0.92
(1,313)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	6	0.92
(1,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	10	0.92
(1,291)	1:21:A:ARG:HA	1:22:A:PRO:HD2	3	0.92
(1,291)	1:21:A:ARG:HA	1:22:A:PRO:HD2	4	0.92
(1,291)	1:21:A:ARG:HA	1:22:A:PRO:HD2	9	0.92
(1,279)	1:19:A:SER:H	1:20:A:GLY:H	3	0.92
(4,3)	1:22:A:PRO:HA	1:22:A:PRO:HD3	6	0.91
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	5	0.91
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	5	0.91
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	5	0.91
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	5	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	5	0.91
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	5	0.91
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	5	0.91
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	5	0.91
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	5	0.91
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	5	0.91
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	5	0.91
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	5	0.91
(2,51)	1:22:A:PRO:HA	1:22:A:PRO:HD3	6	0.91
(1,309)	1:9:A:ILE:HA	1:12:A:LEU:HB2	10	0.91
(1,279)	1:19:A:SER:H	1:20:A:GLY:H	1	0.91
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	5	0.91
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	5	0.91
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	5	0.91
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	6	0.91
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	6	0.91
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	6	0.91
(1,116)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	2	0.91
(1,80)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	9	0.91
(1,61)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	1	0.91
(1,61)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	10	0.91
(1,21)	1:15:A:GLY:H	1:15:A:GLY:HA2	10	0.91
(1,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	9	0.9
(1,288)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	1	0.9
(1,288)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	1	0.9
(1,288)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	6	0.9
(1,288)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	6	0.9
(1,247)	1:21:A:ARG:H	1:21:A:ARG:HG2	3	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	2	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	2	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	2	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	3	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	3	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	3	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	8	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	8	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	8	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	9	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	9	0.9
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	9	0.9
(1,61)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	8	0.9
(1,309)	1:9:A:ILE:HA	1:12:A:LEU:HB2	4	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:9:A:ILE:HA	1:12:A:LEU:HB2	5	0.89
(1,309)	1:9:A:ILE:HA	1:12:A:LEU:HB2	7	0.89
(1,284)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	5	0.89
(1,279)	1:19:A:SER:H	1:20:A:GLY:H	9	0.89
(1,269)	1:19:A:SER:H	1:19:A:SER:HB2	1	0.89
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	7	0.89
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	7	0.89
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	7	0.89
(1,70)	1:23:A:PRO:HA	1:23:A:PRO:HB3	6	0.89
(1,61)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	2	0.89
(1,326)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	1	0.88
(1,326)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	1	0.88
(1,326)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	1	0.88
(1,326)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	1	0.88
(1,326)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	1	0.88
(1,326)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	1	0.88
(1,320)	1:16:A:GLY:HA2	1:21:A:ARG:HB2	3	0.88
(1,320)	1:16:A:GLY:HA2	1:21:A:ARG:HB2	4	0.88
(1,320)	1:16:A:GLY:HA2	1:21:A:ARG:HB2	9	0.88
(1,315)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	2	0.88
(1,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	5	0.88
(1,283)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	7	0.88
(1,89)	1:24:A:PRO:HA	1:24:A:PRO:HB3	8	0.88
(1,70)	1:23:A:PRO:HA	1:23:A:PRO:HB3	1	0.88
(1,70)	1:23:A:PRO:HA	1:23:A:PRO:HB3	2	0.88
(1,70)	1:23:A:PRO:HA	1:23:A:PRO:HB3	3	0.88
(1,70)	1:23:A:PRO:HA	1:23:A:PRO:HB3	5	0.88
(1,70)	1:23:A:PRO:HA	1:23:A:PRO:HB3	7	0.88
(1,70)	1:23:A:PRO:HA	1:23:A:PRO:HB3	9	0.88
(1,70)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.88
(1,309)	1:9:A:ILE:HA	1:12:A:LEU:HB2	6	0.87
(1,247)	1:21:A:ARG:H	1:21:A:ARG:HG2	2	0.87
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	10	0.87
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	10	0.87
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	10	0.87
(1,104)	1:10:A:GLN:H	1:10:A:GLN:HG3	5	0.87
(1,70)	1:23:A:PRO:HA	1:23:A:PRO:HB3	8	0.87
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.86
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.86
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.86
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.86
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.86
(1,309)	1:9:A:ILE:HA	1:12:A:LEU:HB2	8	0.86
(1,288)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	7	0.86
(1,288)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	7	0.86
(1,269)	1:19:A:SER:H	1:19:A:SER:HB2	4	0.86
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	1	0.86
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	1	0.86
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	1	0.86
(1,61)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	7	0.86
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	6	0.85
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	6	0.85
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	6	0.85
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD11	6	0.85
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD12	6	0.85
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD13	6	0.85
(1,334)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	6	0.85
(1,334)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	6	0.85
(1,334)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	6	0.85
(1,334)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	6	0.85
(1,334)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	6	0.85
(1,334)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	6	0.85
(1,283)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	10	0.85
(1,279)	1:19:A:SER:H	1:20:A:GLY:H	4	0.85
(1,279)	1:19:A:SER:H	1:20:A:GLY:H	7	0.85
(1,260)	1:4:A:ALA:HB1	1:5:A:VAL:H	7	0.85
(1,260)	1:4:A:ALA:HB2	1:5:A:VAL:H	7	0.85
(1,260)	1:4:A:ALA:HB3	1:5:A:VAL:H	7	0.85
(1,104)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.85
(1,89)	1:24:A:PRO:HA	1:24:A:PRO:HB3	1	0.85
(1,89)	1:24:A:PRO:HA	1:24:A:PRO:HB3	3	0.85
(1,89)	1:24:A:PRO:HA	1:24:A:PRO:HB3	9	0.85
(1,89)	1:24:A:PRO:HA	1:24:A:PRO:HB3	10	0.85
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	10	0.85
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	10	0.85
(3,306)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	6	0.84
(2,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	6	0.84
(1,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	6	0.84
(1,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	0.84
(1,309)	1:9:A:ILE:HA	1:12:A:LEU:HB2	3	0.84
(1,286)	1:21:A:ARG:H	1:21:A:ARG:HB2	1	0.84
(1,267)	1:18:A:SER:H	1:18:A:SER:HB2	6	0.84
(1,267)	1:18:A:SER:H	1:18:A:SER:HB3	6	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,109)	1:6:A:ARG:H	1:6:A:ARG:HB3	7	0.84
(1,89)	1:24:A:PRO:HA	1:24:A:PRO:HB3	2	0.84
(1,84)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	2	0.84
(1,80)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	0.84
(1,70)	1:23:A:PRO:HA	1:23:A:PRO:HB3	4	0.84
(1,24)	1:25:A:SER:H	1:25:A:SER:HB2	8	0.84
(1,24)	1:25:A:SER:H	1:25:A:SER:HB3	8	0.84
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	7	0.83
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	7	0.83
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	7	0.83
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD11	7	0.83
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD12	7	0.83
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD13	7	0.83
(1,288)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	9	0.83
(1,288)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	9	0.83
(1,285)	1:3:A:GLU:HB2	1:4:A:ALA:H	7	0.83
(1,267)	1:18:A:SER:H	1:18:A:SER:HB2	5	0.83
(1,267)	1:18:A:SER:H	1:18:A:SER:HB3	5	0.83
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	3	0.83
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	3	0.83
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	3	0.83
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	3	0.83
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	3	0.83
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	3	0.83
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	3	0.83
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	3	0.83
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	3	0.83
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	3	0.83
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	3	0.83
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	3	0.83
(1,115)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	6	0.83
(1,109)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.83
(1,84)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	3	0.83
(1,84)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	8	0.83
(1,324)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	5	0.82
(1,324)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	5	0.82
(1,324)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	5	0.82
(1,324)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	5	0.82
(1,324)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	5	0.82
(1,324)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	5	0.82
(1,304)	1:3:A:GLU:HA	1:6:A:ARG:HB3	6	0.82
(1,118)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:24:A:PRO:HA	1:24:A:PRO:HB3	5	0.82
(1,84)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	1	0.82
(1,84)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.82
(1,18)	1:19:A:SER:H	1:19:A:SER:HA	6	0.82
(1,320)	1:16:A:GLY:HA2	1:21:A:ARG:HB2	1	0.81
(1,309)	1:9:A:ILE:HA	1:12:A:LEU:HB2	2	0.81
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	6	0.81
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	6	0.81
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	6	0.81
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	6	0.81
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	6	0.81
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	6	0.81
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	6	0.81
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	6	0.81
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	6	0.81
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	6	0.81
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	6	0.81
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	6	0.81
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	4	0.81
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	4	0.81
(1,203)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	4	0.81
(1,139)	1:5:A:VAL:H	1:6:A:ARG:H	10	0.81
(1,115)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	10	0.81
(1,109)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.81
(1,89)	1:24:A:PRO:HA	1:24:A:PRO:HB3	6	0.81
(1,84)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	5	0.81
(1,80)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	1	0.81
(1,61)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.81
(1,320)	1:16:A:GLY:HA2	1:21:A:ARG:HB2	5	0.8
(1,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.8
(1,24)	1:25:A:SER:H	1:25:A:SER:HB2	9	0.8
(1,24)	1:25:A:SER:H	1:25:A:SER:HB3	9	0.8
(1,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	0.79
(1,288)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	3	0.79
(1,288)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	3	0.79
(1,84)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	6	0.79
(1,84)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	9	0.79
(1,21)	1:15:A:GLY:H	1:15:A:GLY:HA2	9	0.79
(1,16)	1:8:A:TYR:H	1:8:A:TYR:HB3	10	0.79
(3,214)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.78
(2,221)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.78
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD11	9	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD12	9	0.78
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD13	9	0.78
(1,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	0.78
(1,141)	1:7:A:LEU:H	1:8:A:TYR:H	2	0.78
(1,87)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	7	0.78
(1,18)	1:19:A:SER:H	1:19:A:SER:HA	2	0.78
(1,286)	1:21:A:ARG:H	1:21:A:ARG:HB2	9	0.77
(1,206)	1:12:A:LEU:HD11	1:12:A:LEU:HG	1	0.77
(1,206)	1:12:A:LEU:HD12	1:12:A:LEU:HG	1	0.77
(1,206)	1:12:A:LEU:HD13	1:12:A:LEU:HG	1	0.77
(1,206)	1:12:A:LEU:HD11	1:12:A:LEU:HG	2	0.77
(1,206)	1:12:A:LEU:HD12	1:12:A:LEU:HG	2	0.77
(1,206)	1:12:A:LEU:HD13	1:12:A:LEU:HG	2	0.77
(1,206)	1:12:A:LEU:HD11	1:12:A:LEU:HG	3	0.77
(1,206)	1:12:A:LEU:HD12	1:12:A:LEU:HG	3	0.77
(1,206)	1:12:A:LEU:HD13	1:12:A:LEU:HG	3	0.77
(1,206)	1:12:A:LEU:HD11	1:12:A:LEU:HG	7	0.77
(1,206)	1:12:A:LEU:HD12	1:12:A:LEU:HG	7	0.77
(1,206)	1:12:A:LEU:HD13	1:12:A:LEU:HG	7	0.77
(1,119)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	5	0.77
(1,119)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	8	0.77
(1,119)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	9	0.77
(1,114)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	2	0.77
(1,84)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	4	0.77
(4,15)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	8	0.76
(3,214)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.76
(3,214)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	0.76
(3,214)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.76
(3,214)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.76
(2,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	8	0.76
(2,221)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.76
(2,221)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	0.76
(2,221)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.76
(2,221)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.76
(1,331)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	5	0.76
(1,331)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	5	0.76
(1,331)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	5	0.76
(1,279)	1:19:A:SER:H	1:20:A:GLY:H	2	0.76
(1,255)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	6	0.76
(1,255)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	6	0.76
(1,252)	1:5:A:VAL:HG11	1:6:A:ARG:H	6	0.76
(1,252)	1:5:A:VAL:HG12	1:6:A:ARG:H	6	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:5:A:VAL:HG13	1:6:A:ARG:H	6	0.76
(1,252)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.76
(1,252)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.76
(1,252)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.76
(1,206)	1:12:A:LEU:HD11	1:12:A:LEU:HG	5	0.76
(1,206)	1:12:A:LEU:HD12	1:12:A:LEU:HG	5	0.76
(1,206)	1:12:A:LEU:HD13	1:12:A:LEU:HG	5	0.76
(1,206)	1:12:A:LEU:HD11	1:12:A:LEU:HG	6	0.76
(1,206)	1:12:A:LEU:HD12	1:12:A:LEU:HG	6	0.76
(1,206)	1:12:A:LEU:HD13	1:12:A:LEU:HG	6	0.76
(1,206)	1:12:A:LEU:HD11	1:12:A:LEU:HG	8	0.76
(1,206)	1:12:A:LEU:HD12	1:12:A:LEU:HG	8	0.76
(1,206)	1:12:A:LEU:HD13	1:12:A:LEU:HG	8	0.76
(1,206)	1:12:A:LEU:HD11	1:12:A:LEU:HG	9	0.76
(1,206)	1:12:A:LEU:HD12	1:12:A:LEU:HG	9	0.76
(1,206)	1:12:A:LEU:HD13	1:12:A:LEU:HG	9	0.76
(1,206)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.76
(1,206)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.76
(1,206)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.76
(1,134)	1:14:A:GLN:H	1:14:A:GLN:HG3	2	0.76
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	3	0.76
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	3	0.76
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	7	0.76
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	7	0.76
(1,119)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	1	0.76
(1,24)	1:25:A:SER:H	1:25:A:SER:HB2	5	0.76
(1,24)	1:25:A:SER:H	1:25:A:SER:HB3	5	0.76
(1,18)	1:19:A:SER:H	1:19:A:SER:HA	7	0.76
(1,18)	1:19:A:SER:H	1:19:A:SER:HA	9	0.76
(1,16)	1:8:A:TYR:H	1:8:A:TYR:HB3	3	0.76
(3,247)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	1	0.75
(3,247)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	1	0.75
(3,247)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	6	0.75
(3,247)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	6	0.75
(3,214)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.75
(3,214)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.75
(3,214)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.75
(3,214)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	0.75
(2,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	1	0.75
(2,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	1	0.75
(2,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	6	0.75
(2,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	6	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,221)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.75
(2,221)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.75
(2,221)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.75
(2,221)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	0.75
(1,335)	1:7:A:LEU:HD11	1:8:A:TYR:HB2	1	0.75
(1,335)	1:7:A:LEU:HD12	1:8:A:TYR:HB2	1	0.75
(1,335)	1:7:A:LEU:HD13	1:8:A:TYR:HB2	1	0.75
(1,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	4	0.75
(1,315)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	10	0.75
(1,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	0.75
(1,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.75
(1,104)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.75
(1,84)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	7	0.75
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	2	0.75
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	2	0.75
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD2	1	0.75
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD3	1	0.75
(1,24)	1:25:A:SER:H	1:25:A:SER:HB2	1	0.75
(1,24)	1:25:A:SER:H	1:25:A:SER:HB3	1	0.75
(1,18)	1:19:A:SER:H	1:19:A:SER:HA	3	0.75
(1,18)	1:19:A:SER:H	1:19:A:SER:HA	4	0.75
(3,214)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.74
(3,188)	1:12:A:LEU:HA	1:12:A:LEU:HD11	4	0.74
(3,188)	1:12:A:LEU:HA	1:12:A:LEU:HD12	4	0.74
(3,188)	1:12:A:LEU:HA	1:12:A:LEU:HD13	4	0.74
(2,221)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.74
(2,195)	1:12:A:LEU:HA	1:12:A:LEU:HD11	4	0.74
(2,195)	1:12:A:LEU:HA	1:12:A:LEU:HD12	4	0.74
(2,195)	1:12:A:LEU:HA	1:12:A:LEU:HD13	4	0.74
(1,337)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	2	0.74
(1,337)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	2	0.74
(1,337)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	2	0.74
(1,335)	1:7:A:LEU:HD11	1:8:A:TYR:HB2	10	0.74
(1,335)	1:7:A:LEU:HD12	1:8:A:TYR:HB2	10	0.74
(1,335)	1:7:A:LEU:HD13	1:8:A:TYR:HB2	10	0.74
(1,260)	1:4:A:ALA:HB1	1:5:A:VAL:H	6	0.74
(1,260)	1:4:A:ALA:HB2	1:5:A:VAL:H	6	0.74
(1,260)	1:4:A:ALA:HB3	1:5:A:VAL:H	6	0.74
(1,158)	1:7:A:LEU:HB3	1:7:A:LEU:HG	6	0.74
(1,158)	1:7:A:LEU:HB3	1:7:A:LEU:HG	7	0.74
(1,139)	1:5:A:VAL:H	1:6:A:ARG:H	6	0.74
(1,119)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	7	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD2	6	0.74
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD3	6	0.74
(1,18)	1:19:A:SER:H	1:19:A:SER:HA	1	0.74
(1,16)	1:8:A:TYR:H	1:8:A:TYR:HB3	1	0.74
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	3	0.73
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	3	0.73
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	3	0.73
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	3	0.73
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	3	0.73
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	3	0.73
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	3	0.73
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	3	0.73
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	3	0.73
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	8	0.73
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	8	0.73
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	8	0.73
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	8	0.73
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	8	0.73
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	8	0.73
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	3	0.73
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	3	0.73
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	3	0.73
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	3	0.73
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	3	0.73
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	3	0.73
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	3	0.73
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	3	0.73
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	3	0.73
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	8	0.73
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	8	0.73
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	8	0.73
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	8	0.73
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	8	0.73
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	8	0.73
(1,332)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	6	0.73
(1,332)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	6	0.73
(1,332)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	6	0.73
(1,291)	1:21:A:ARG:HA	1:22:A:PRO:HD2	5	0.73
(1,239)	1:3:A:GLU:HB3	1:4:A:ALA:H	10	0.73
(1,206)	1:12:A:LEU:HD11	1:12:A:LEU:HG	4	0.73
(1,206)	1:12:A:LEU:HD12	1:12:A:LEU:HG	4	0.73
(1,206)	1:12:A:LEU:HD13	1:12:A:LEU:HG	4	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:14:A:GLN:H	1:14:A:GLN:HG2	1	0.73
(1,16)	1:8:A:TYR:H	1:8:A:TYR:HB3	9	0.73
(1,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	2	0.72
(1,269)	1:19:A:SER:H	1:19:A:SER:HB2	2	0.72
(1,223)	1:15:A:GLY:H	1:16:A:GLY:H	10	0.72
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	10	0.72
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	10	0.72
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	10	0.72
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	10	0.72
(1,165)	1:7:A:LEU:H	1:7:A:LEU:HG	6	0.72
(1,141)	1:7:A:LEU:H	1:8:A:TYR:H	4	0.72
(1,129)	1:14:A:GLN:HA	1:14:A:GLN:HG2	4	0.72
(1,110)	1:6:A:ARG:H	1:6:A:ARG:HG3	3	0.72
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.71
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.71
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.71
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.71
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.71
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.71
(1,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	0.71
(1,269)	1:19:A:SER:H	1:19:A:SER:HB2	9	0.71
(1,245)	1:7:A:LEU:HB2	1:8:A:TYR:H	9	0.71
(1,80)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	2	0.71
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD2	3	0.71
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD3	3	0.71
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	6	0.71
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	6	0.71
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	8	0.71
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	8	0.71
(1,31)	1:17:A:PRO:HA	1:17:A:PRO:HB3	2	0.71
(1,24)	1:25:A:SER:H	1:25:A:SER:HB2	6	0.71
(1,24)	1:25:A:SER:H	1:25:A:SER:HB3	6	0.71
(1,24)	1:25:A:SER:H	1:25:A:SER:HB2	7	0.71
(1,24)	1:25:A:SER:H	1:25:A:SER:HB3	7	0.71
(3,232)	1:6:A:ARG:HB3	1:7:A:LEU:H	9	0.7
(2,242)	1:6:A:ARG:HB3	1:7:A:LEU:H	9	0.7
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	3	0.7
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	3	0.7
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	3	0.7
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	3	0.7
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	7	0.7
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	7	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	7	0.7
(1,104)	1:10:A:GLN:H	1:10:A:GLN:HG3	1	0.7
(1,80)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	3	0.7
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD2	5	0.7
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD3	5	0.7
(1,31)	1:17:A:PRO:HA	1:17:A:PRO:HB3	4	0.7
(1,31)	1:17:A:PRO:HA	1:17:A:PRO:HB3	7	0.7
(1,24)	1:25:A:SER:H	1:25:A:SER:HB2	2	0.7
(1,24)	1:25:A:SER:H	1:25:A:SER:HB3	2	0.7
(1,24)	1:25:A:SER:H	1:25:A:SER:HB2	3	0.7
(1,24)	1:25:A:SER:H	1:25:A:SER:HB3	3	0.7
(1,326)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	8	0.69
(1,326)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	8	0.69
(1,326)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	8	0.69
(1,326)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	8	0.69
(1,326)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	8	0.69
(1,326)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	8	0.69
(1,273)	1:13:A:LYS:H	1:14:A:GLN:H	6	0.69
(1,158)	1:7:A:LEU:HB3	1:7:A:LEU:HG	2	0.69
(1,158)	1:7:A:LEU:HB3	1:7:A:LEU:HG	9	0.69
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG2	8	0.69
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG3	8	0.69
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG11	5	0.69
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG12	5	0.69
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG13	5	0.69
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG21	5	0.69
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG22	5	0.69
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG23	5	0.69
(1,134)	1:14:A:GLN:H	1:14:A:GLN:HG3	4	0.69
(1,129)	1:14:A:GLN:HA	1:14:A:GLN:HG2	9	0.69
(1,83)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	7	0.69
(1,67)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	1	0.69
(1,67)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	1	0.69
(1,67)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	4	0.69
(1,67)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	4	0.69
(1,67)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	5	0.69
(1,67)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	5	0.69
(1,67)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	8	0.69
(1,67)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	8	0.69
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	9	0.69
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	9	0.69
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD2	9	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD3	9	0.69
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	1	0.69
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	1	0.69
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	10	0.69
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	10	0.69
(1,31)	1:17:A:PRO:HA	1:17:A:PRO:HB3	1	0.69
(1,31)	1:17:A:PRO:HA	1:17:A:PRO:HB3	3	0.69
(1,31)	1:17:A:PRO:HA	1:17:A:PRO:HB3	5	0.69
(1,31)	1:17:A:PRO:HA	1:17:A:PRO:HB3	9	0.69
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	7	0.68
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	7	0.68
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	7	0.68
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	7	0.68
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	7	0.68
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	7	0.68
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	7	0.68
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	7	0.68
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	7	0.68
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	7	0.68
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	7	0.68
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	7	0.68
(1,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	8	0.68
(1,194)	1:20:A:GLY:H	1:20:A:GLY:HA3	5	0.68
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG2	10	0.68
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG3	10	0.68
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG11	2	0.68
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG12	2	0.68
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG13	2	0.68
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG21	2	0.68
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG22	2	0.68
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG23	2	0.68
(1,141)	1:7:A:LEU:H	1:8:A:TYR:H	8	0.68
(1,67)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	2	0.68
(1,67)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	2	0.68
(1,67)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	3	0.68
(1,67)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	3	0.68
(1,67)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	7	0.68
(1,67)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	7	0.68
(1,67)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	9	0.68
(1,67)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	9	0.68
(1,67)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	10	0.68
(1,67)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	6	0.68
(1,66)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	6	0.68
(1,42)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	7	0.68
(1,42)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	7	0.68
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	3	0.68
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	3	0.68
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	5	0.68
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	5	0.68
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	7	0.68
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	7	0.68
(1,16)	1:8:A:TYR:H	1:8:A:TYR:HB3	4	0.68
(1,16)	1:8:A:TYR:H	1:8:A:TYR:HB3	5	0.68
(1,16)	1:8:A:TYR:H	1:8:A:TYR:HB3	7	0.68
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	10	0.67
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	10	0.67
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	10	0.67
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	10	0.67
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	10	0.67
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	10	0.67
(3,232)	1:6:A:ARG:HB3	1:7:A:LEU:H	1	0.67
(3,159)	1:7:A:LEU:H	1:7:A:LEU:HB2	2	0.67
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	10	0.67
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	10	0.67
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	10	0.67
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	10	0.67
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	10	0.67
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	10	0.67
(2,242)	1:6:A:ARG:HB3	1:7:A:LEU:H	1	0.67
(2,166)	1:7:A:LEU:H	1:7:A:LEU:HB2	2	0.67
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD11	5	0.67
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD12	5	0.67
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD13	5	0.67
(1,320)	1:16:A:GLY:HA2	1:21:A:ARG:HB2	8	0.67
(1,273)	1:13:A:LYS:H	1:14:A:GLN:H	5	0.67
(1,260)	1:4:A:ALA:HB1	1:5:A:VAL:H	2	0.67
(1,260)	1:4:A:ALA:HB2	1:5:A:VAL:H	2	0.67
(1,260)	1:4:A:ALA:HB3	1:5:A:VAL:H	2	0.67
(1,222)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	8	0.67
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	4	0.67
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	4	0.67
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	4	0.67
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	4	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:14:A:GLN:HA	1:14:A:GLN:HG2	6	0.67
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	2	0.67
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	2	0.67
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	9	0.67
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	9	0.67
(1,31)	1:17:A:PRO:HA	1:17:A:PRO:HB3	6	0.67
(3,316)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	7	0.66
(3,316)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	7	0.66
(3,316)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	7	0.66
(2,331)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	7	0.66
(2,331)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	7	0.66
(2,331)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	7	0.66
(1,337)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	4	0.66
(1,337)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	4	0.66
(1,337)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	4	0.66
(1,315)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	3	0.66
(1,286)	1:21:A:ARG:H	1:21:A:ARG:HB2	6	0.66
(1,247)	1:21:A:ARG:H	1:21:A:ARG:HG2	10	0.66
(1,239)	1:3:A:GLU:HB3	1:4:A:ALA:H	2	0.66
(1,222)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	4	0.66
(1,222)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	9	0.66
(1,222)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	0.66
(1,129)	1:14:A:GLN:HA	1:14:A:GLN:HG2	8	0.66
(1,31)	1:17:A:PRO:HA	1:17:A:PRO:HB3	8	0.66
(1,16)	1:8:A:TYR:H	1:8:A:TYR:HB3	6	0.66
(3,159)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.65
(2,166)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.65
(1,335)	1:7:A:LEU:HD11	1:8:A:TYR:HB2	3	0.65
(1,335)	1:7:A:LEU:HD12	1:8:A:TYR:HB2	3	0.65
(1,335)	1:7:A:LEU:HD13	1:8:A:TYR:HB2	3	0.65
(1,329)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	1	0.65
(1,329)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	1	0.65
(1,329)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	1	0.65
(1,286)	1:21:A:ARG:H	1:21:A:ARG:HB2	3	0.65
(1,284)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	8	0.65
(1,224)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	1	0.65
(1,224)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	2	0.65
(1,224)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	3	0.65
(1,224)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	5	0.65
(1,224)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	6	0.65
(1,224)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	7	0.65
(1,224)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.65
(1,222)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	1	0.65
(1,222)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	2	0.65
(1,222)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	5	0.65
(1,222)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	6	0.65
(1,222)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	7	0.65
(1,165)	1:7:A:LEU:H	1:7:A:LEU:HG	7	0.65
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG2	4	0.65
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG3	4	0.65
(1,145)	1:5:A:VAL:HA	1:5:A:VAL:HB	2	0.65
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB2	1	0.65
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB3	1	0.65
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB2	5	0.65
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB3	5	0.65
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD2	7	0.65
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD3	7	0.65
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	1	0.65
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	1	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	1	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	1	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	2	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	2	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	3	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	3	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	4	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	4	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	5	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	5	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	7	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	7	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	9	0.65
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	9	0.65
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	4	0.65
(1,34)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	4	0.65
(3,317)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	10	0.64
(3,317)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	10	0.64
(3,317)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	10	0.64
(3,232)	1:6:A:ARG:HB3	1:7:A:LEU:H	5	0.64
(2,332)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	10	0.64
(2,332)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	10	0.64
(2,332)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	10	0.64
(2,242)	1:6:A:ARG:HB3	1:7:A:LEU:H	5	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	7	0.64
(1,320)	1:16:A:GLY:HA2	1:21:A:ARG:HB2	10	0.64
(1,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	7	0.64
(1,286)	1:21:A:ARG:H	1:21:A:ARG:HB2	2	0.64
(1,227)	1:13:A:LYS:HA	1:14:A:GLN:H	10	0.64
(1,225)	1:16:A:GLY:H	1:16:A:GLY:HA3	2	0.64
(1,225)	1:16:A:GLY:H	1:16:A:GLY:HA3	7	0.64
(1,225)	1:16:A:GLY:H	1:16:A:GLY:HA3	8	0.64
(1,224)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	4	0.64
(1,224)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	8	0.64
(1,222)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	3	0.64
(1,176)	1:9:A:ILE:H	1:9:A:ILE:HG12	6	0.64
(1,176)	1:9:A:ILE:H	1:9:A:ILE:HG12	8	0.64
(1,165)	1:7:A:LEU:H	1:7:A:LEU:HG	8	0.64
(1,145)	1:5:A:VAL:HA	1:5:A:VAL:HB	5	0.64
(1,113)	1:6:A:ARG:HA	1:6:A:ARG:HB2	7	0.64
(1,113)	1:6:A:ARG:HA	1:6:A:ARG:HB2	8	0.64
(1,91)	1:24:A:PRO:HA	1:24:A:PRO:HG3	4	0.64
(1,67)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	6	0.64
(1,67)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	6	0.64
(1,66)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	8	0.64
(1,66)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	8	0.64
(1,55)	1:22:A:PRO:HA	1:22:A:PRO:HB3	7	0.64
(1,55)	1:22:A:PRO:HA	1:22:A:PRO:HB3	8	0.64
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD2	2	0.64
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD3	2	0.64
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	6	0.64
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	6	0.64
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	8	0.64
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	8	0.64
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	5	0.64
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	5	0.64
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	6	0.64
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	6	0.64
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	8	0.64
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	8	0.64
(1,31)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.64
(1,16)	1:8:A:TYR:H	1:8:A:TYR:HB3	8	0.64
(4,3)	1:22:A:PRO:HA	1:22:A:PRO:HD3	5	0.63
(3,159)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.63
(2,166)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.63
(2,51)	1:22:A:PRO:HA	1:22:A:PRO:HD3	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	2	0.63
(1,324)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	2	0.63
(1,324)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	2	0.63
(1,324)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	2	0.63
(1,324)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	2	0.63
(1,324)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	2	0.63
(1,315)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	5	0.63
(1,304)	1:3:A:GLU:HA	1:6:A:ARG:HB3	7	0.63
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	7	0.63
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	7	0.63
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	7	0.63
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	7	0.63
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	7	0.63
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	7	0.63
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	7	0.63
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	7	0.63
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	7	0.63
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	7	0.63
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	7	0.63
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	7	0.63
(1,225)	1:16:A:GLY:H	1:16:A:GLY:HA3	1	0.63
(1,225)	1:16:A:GLY:H	1:16:A:GLY:HA3	3	0.63
(1,225)	1:16:A:GLY:H	1:16:A:GLY:HA3	4	0.63
(1,225)	1:16:A:GLY:H	1:16:A:GLY:HA3	9	0.63
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	2	0.63
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	2	0.63
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	2	0.63
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	2	0.63
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	5	0.63
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	5	0.63
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	5	0.63
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	5	0.63
(1,165)	1:7:A:LEU:H	1:7:A:LEU:HG	4	0.63
(1,148)	1:3:A:GLU:HA	1:3:A:GLU:HB2	9	0.63
(1,116)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	6	0.63
(1,104)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.63
(1,103)	1:10:A:GLN:H	1:10:A:GLN:HG2	7	0.63
(1,78)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	6	0.63
(1,66)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	5	0.63
(1,66)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	5	0.63
(1,55)	1:22:A:PRO:HA	1:22:A:PRO:HB3	1	0.63
(1,55)	1:22:A:PRO:HA	1:22:A:PRO:HB3	2	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:22:A:PRO:HA	1:22:A:PRO:HB3	4	0.63
(1,55)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.63
(1,44)	1:21:A:ARG:HA	1:21:A:ARG:HB3	10	0.63
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	10	0.63
(1,39)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	10	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	1	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	1	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	2	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	2	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	3	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	3	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	7	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	7	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	9	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	9	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.63
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	10	0.63
(3,247)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	2	0.62
(3,247)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	2	0.62
(3,211)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.62
(3,211)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.62
(2,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	2	0.62
(2,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	2	0.62
(2,218)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.62
(2,218)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.62
(1,304)	1:3:A:GLU:HA	1:6:A:ARG:HB3	8	0.62
(1,296)	1:8:A:TYR:HA	1:24:A:PRO:HD3	7	0.62
(1,225)	1:16:A:GLY:H	1:16:A:GLY:HA3	10	0.62
(1,176)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.62
(1,141)	1:7:A:LEU:H	1:8:A:TYR:H	7	0.62
(1,139)	1:5:A:VAL:H	1:6:A:ARG:H	8	0.62
(1,109)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.62
(1,104)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.62
(1,103)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.62
(1,78)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	1	0.62
(1,78)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	2	0.62
(1,78)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	5	0.62
(1,78)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	7	0.62
(1,78)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	8	0.62
(1,78)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	9	0.62
(1,78)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	10	0.62
(1,66)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	1	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	1	0.62
(1,66)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	2	0.62
(1,66)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	2	0.62
(1,66)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	3	0.62
(1,66)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	3	0.62
(1,66)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	4	0.62
(1,66)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	4	0.62
(1,66)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	9	0.62
(1,66)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	9	0.62
(1,66)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.62
(1,66)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	10	0.62
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD2	6	0.62
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD3	6	0.62
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD2	10	0.62
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.62
(1,55)	1:22:A:PRO:HA	1:22:A:PRO:HB3	3	0.62
(1,55)	1:22:A:PRO:HA	1:22:A:PRO:HB3	9	0.62
(1,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	5	0.62
(1,38)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	1	0.62
(1,38)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	2	0.62
(1,38)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	3	0.62
(1,38)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	4	0.62
(1,38)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	5	0.62
(1,38)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	6	0.62
(1,38)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	7	0.62
(1,38)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	8	0.62
(1,38)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	9	0.62
(1,38)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.62
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	4	0.62
(1,36)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	4	0.62
(3,315)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	7	0.61
(3,315)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	7	0.61
(3,315)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	7	0.61
(3,211)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.61
(3,211)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.61
(2,330)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	7	0.61
(2,330)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	7	0.61
(2,330)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	7	0.61
(2,218)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.61
(2,218)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.61
(1,334)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	8	0.61
(1,334)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	8	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	8	0.61
(1,334)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	8	0.61
(1,334)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	8	0.61
(1,334)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	8	0.61
(1,315)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	9	0.61
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB2	3	0.61
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB3	3	0.61
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB2	9	0.61
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB3	9	0.61
(1,273)	1:13:A:LYS:H	1:14:A:GLN:H	7	0.61
(1,238)	1:3:A:GLU:H	1:3:A:GLU:HB2	8	0.61
(1,231)	1:11:A:TRP:HB3	1:12:A:LEU:H	3	0.61
(1,225)	1:16:A:GLY:H	1:16:A:GLY:HA3	5	0.61
(1,194)	1:20:A:GLY:H	1:20:A:GLY:HA3	8	0.61
(1,121)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	8	0.61
(1,113)	1:6:A:ARG:HA	1:6:A:ARG:HB2	10	0.61
(1,78)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	3	0.61
(1,66)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	7	0.61
(1,66)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	7	0.61
(1,55)	1:22:A:PRO:HA	1:22:A:PRO:HB3	6	0.61
(1,20)	1:2:A:GLU:HA	1:3:A:GLU:H	7	0.61
(3,316)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	8	0.6
(3,316)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	8	0.6
(3,316)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	8	0.6
(3,211)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.6
(3,211)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.6
(2,331)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	8	0.6
(2,331)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	8	0.6
(2,331)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	8	0.6
(2,218)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.6
(2,218)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.6
(1,313)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	9	0.6
(1,284)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	3	0.6
(1,176)	1:9:A:ILE:H	1:9:A:ILE:HG12	3	0.6
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	2	0.6
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	2	0.6
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	2	0.6
(1,145)	1:5:A:VAL:HA	1:5:A:VAL:HB	3	0.6
(1,141)	1:7:A:LEU:H	1:8:A:TYR:H	6	0.6
(1,134)	1:14:A:GLN:H	1:14:A:GLN:HG3	6	0.6
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	1	0.6
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	1	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	1	0.6
(1,121)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	5	0.6
(1,119)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	3	0.6
(1,119)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	4	0.6
(1,79)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	1	0.6
(1,79)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	2	0.6
(1,79)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	4	0.6
(1,79)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	6	0.6
(1,79)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	7	0.6
(1,79)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	8	0.6
(1,78)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	4	0.6
(1,72)	1:23:A:PRO:HA	1:23:A:PRO:HG3	10	0.6
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	4	0.6
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	4	0.6
(3,211)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.59
(3,211)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.59
(3,211)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.59
(2,218)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.59
(2,218)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.59
(2,218)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.59
(1,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	8	0.59
(1,269)	1:19:A:SER:H	1:19:A:SER:HB2	3	0.59
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	5	0.59
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	5	0.59
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	5	0.59
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	5	0.59
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	5	0.59
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	5	0.59
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	5	0.59
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	5	0.59
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	5	0.59
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	5	0.59
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	5	0.59
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	5	0.59
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	6	0.59
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	6	0.59
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	6	0.59
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	6	0.59
(1,145)	1:5:A:VAL:HA	1:5:A:VAL:HB	8	0.59
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	9	0.59
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	9	0.59
(1,129)	1:14:A:GLN:HA	1:14:A:GLN:HG2	2	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:14:A:GLN:HA	1:14:A:GLN:HG2	10	0.59
(1,121)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	7	0.59
(1,121)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	9	0.59
(1,113)	1:6:A:ARG:HA	1:6:A:ARG:HB2	6	0.59
(1,79)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	3	0.59
(1,79)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	5	0.59
(1,79)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	9	0.59
(1,79)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.59
(1,72)	1:23:A:PRO:HA	1:23:A:PRO:HG3	9	0.59
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD2	2	0.59
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD3	2	0.59
(1,20)	1:2:A:GLU:HA	1:3:A:GLU:H	3	0.59
(3,211)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.58
(2,218)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.58
(1,329)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	3	0.58
(1,329)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	3	0.58
(1,329)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	3	0.58
(1,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	7	0.58
(1,225)	1:16:A:GLY:H	1:16:A:GLY:HA3	6	0.58
(1,176)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.58
(1,176)	1:9:A:ILE:H	1:9:A:ILE:HG12	4	0.58
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	3	0.58
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	3	0.58
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	3	0.58
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	6	0.58
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	6	0.58
(1,72)	1:23:A:PRO:HA	1:23:A:PRO:HG3	1	0.58
(1,72)	1:23:A:PRO:HA	1:23:A:PRO:HG3	2	0.58
(1,72)	1:23:A:PRO:HA	1:23:A:PRO:HG3	5	0.58
(1,55)	1:22:A:PRO:HA	1:22:A:PRO:HB3	5	0.58
(1,322)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	6	0.57
(1,284)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	1	0.57
(1,273)	1:13:A:LYS:H	1:14:A:GLN:H	3	0.57
(1,238)	1:3:A:GLU:H	1:3:A:GLU:HB2	2	0.57
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	9	0.57
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	9	0.57
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	9	0.57
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	9	0.57
(1,205)	1:12:A:LEU:HD21	1:12:A:LEU:HG	1	0.57
(1,205)	1:12:A:LEU:HD22	1:12:A:LEU:HG	1	0.57
(1,205)	1:12:A:LEU:HD23	1:12:A:LEU:HG	1	0.57
(1,205)	1:12:A:LEU:HD21	1:12:A:LEU:HG	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:12:A:LEU:HD22	1:12:A:LEU:HG	4	0.57
(1,205)	1:12:A:LEU:HD23	1:12:A:LEU:HG	4	0.57
(1,205)	1:12:A:LEU:HD21	1:12:A:LEU:HG	5	0.57
(1,205)	1:12:A:LEU:HD22	1:12:A:LEU:HG	5	0.57
(1,205)	1:12:A:LEU:HD23	1:12:A:LEU:HG	5	0.57
(1,205)	1:12:A:LEU:HD21	1:12:A:LEU:HG	6	0.57
(1,205)	1:12:A:LEU:HD22	1:12:A:LEU:HG	6	0.57
(1,205)	1:12:A:LEU:HD23	1:12:A:LEU:HG	6	0.57
(1,205)	1:12:A:LEU:HD21	1:12:A:LEU:HG	7	0.57
(1,205)	1:12:A:LEU:HD22	1:12:A:LEU:HG	7	0.57
(1,205)	1:12:A:LEU:HD23	1:12:A:LEU:HG	7	0.57
(1,205)	1:12:A:LEU:HD21	1:12:A:LEU:HG	8	0.57
(1,205)	1:12:A:LEU:HD22	1:12:A:LEU:HG	8	0.57
(1,205)	1:12:A:LEU:HD23	1:12:A:LEU:HG	8	0.57
(1,205)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.57
(1,205)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.57
(1,205)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.57
(1,199)	1:12:A:LEU:HA	1:12:A:LEU:HG	4	0.57
(1,177)	1:9:A:ILE:H	1:9:A:ILE:HG13	2	0.57
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	1	0.57
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	1	0.57
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	1	0.57
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	10	0.57
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	10	0.57
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	10	0.57
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG2	2	0.57
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG3	2	0.57
(1,145)	1:5:A:VAL:HA	1:5:A:VAL:HB	4	0.57
(1,145)	1:5:A:VAL:HA	1:5:A:VAL:HB	7	0.57
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	4	0.57
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	4	0.57
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	5	0.57
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	5	0.57
(1,98)	1:10:A:GLN:HA	1:10:A:GLN:HG2	10	0.57
(1,72)	1:23:A:PRO:HA	1:23:A:PRO:HG3	3	0.57
(1,72)	1:23:A:PRO:HA	1:23:A:PRO:HG3	7	0.57
(1,71)	1:23:A:PRO:HA	1:23:A:PRO:HB2	4	0.57
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD2	3	0.57
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD3	3	0.57
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD2	8	0.57
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD3	8	0.57
(1,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	3	0.56
(1,296)	1:8:A:TYR:HA	1:24:A:PRO:HD3	2	0.56
(1,296)	1:8:A:TYR:HA	1:24:A:PRO:HD3	6	0.56
(1,247)	1:21:A:ARG:H	1:21:A:ARG:HG2	9	0.56
(1,223)	1:15:A:GLY:H	1:16:A:GLY:H	2	0.56
(1,205)	1:12:A:LEU:HD21	1:12:A:LEU:HG	2	0.56
(1,205)	1:12:A:LEU:HD22	1:12:A:LEU:HG	2	0.56
(1,205)	1:12:A:LEU:HD23	1:12:A:LEU:HG	2	0.56
(1,205)	1:12:A:LEU:HD21	1:12:A:LEU:HG	3	0.56
(1,205)	1:12:A:LEU:HD22	1:12:A:LEU:HG	3	0.56
(1,205)	1:12:A:LEU:HD23	1:12:A:LEU:HG	3	0.56
(1,205)	1:12:A:LEU:HD21	1:12:A:LEU:HG	9	0.56
(1,205)	1:12:A:LEU:HD22	1:12:A:LEU:HG	9	0.56
(1,205)	1:12:A:LEU:HD23	1:12:A:LEU:HG	9	0.56
(1,165)	1:7:A:LEU:H	1:7:A:LEU:HG	9	0.56
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	6	0.56
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	6	0.56
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	6	0.56
(1,162)	1:7:A:LEU:HD21	1:7:A:LEU:HG	2	0.56
(1,162)	1:7:A:LEU:HD22	1:7:A:LEU:HG	2	0.56
(1,162)	1:7:A:LEU:HD23	1:7:A:LEU:HG	2	0.56
(1,148)	1:3:A:GLU:HA	1:3:A:GLU:HB2	5	0.56
(1,145)	1:5:A:VAL:HA	1:5:A:VAL:HB	10	0.56
(1,72)	1:23:A:PRO:HA	1:23:A:PRO:HG3	8	0.56
(1,16)	1:8:A:TYR:H	1:8:A:TYR:HB3	2	0.56
(3,259)	1:19:A:SER:HA	1:19:A:SER:HB3	2	0.55
(3,259)	1:19:A:SER:HA	1:19:A:SER:HB3	3	0.55
(3,259)	1:19:A:SER:HA	1:19:A:SER:HB3	9	0.55
(2,272)	1:19:A:SER:HA	1:19:A:SER:HB3	2	0.55
(2,272)	1:19:A:SER:HA	1:19:A:SER:HB3	3	0.55
(2,272)	1:19:A:SER:HA	1:19:A:SER:HB3	9	0.55
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	8	0.55
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	8	0.55
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	8	0.55
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	8	0.55
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	8	0.55
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	8	0.55
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	8	0.55
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	8	0.55
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	8	0.55
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	8	0.55
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	8	0.55
(1,239)	1:3:A:GLU:HB3	1:4:A:ALA:H	3	0.55
(1,231)	1:11:A:TRP:HB3	1:12:A:LEU:H	6	0.55
(1,231)	1:11:A:TRP:HB3	1:12:A:LEU:H	10	0.55
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	1	0.55
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	1	0.55
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	1	0.55
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	5	0.55
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	5	0.55
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	5	0.55
(1,162)	1:7:A:LEU:HD21	1:7:A:LEU:HG	7	0.55
(1,162)	1:7:A:LEU:HD22	1:7:A:LEU:HG	7	0.55
(1,162)	1:7:A:LEU:HD23	1:7:A:LEU:HG	7	0.55
(1,134)	1:14:A:GLN:H	1:14:A:GLN:HG3	10	0.55
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	8	0.55
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	8	0.55
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	10	0.55
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	10	0.55
(1,98)	1:10:A:GLN:HA	1:10:A:GLN:HG2	2	0.55
(1,68)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	6	0.55
(1,68)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	6	0.55
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	6	0.54
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	6	0.54
(3,308)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	6	0.54
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	6	0.54
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	6	0.54
(3,308)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	6	0.54
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	6	0.54
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	6	0.54
(3,308)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	6	0.54
(3,247)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	10	0.54
(3,247)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	10	0.54
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	6	0.54
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	6	0.54
(2,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	6	0.54
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	6	0.54
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	6	0.54
(2,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	6	0.54
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	6	0.54
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	6	0.54
(2,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	6	0.54
(2,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	10	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	10	0.54
(1,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	7	0.54
(1,292)	1:21:A:ARG:HA	1:22:A:PRO:HD3	5	0.54
(1,286)	1:21:A:ARG:H	1:21:A:ARG:HB2	7	0.54
(1,261)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	0.54
(1,231)	1:11:A:TRP:HB3	1:12:A:LEU:H	1	0.54
(1,231)	1:11:A:TRP:HB3	1:12:A:LEU:H	8	0.54
(1,165)	1:7:A:LEU:H	1:7:A:LEU:HG	1	0.54
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG2	7	0.54
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG3	7	0.54
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG11	8	0.54
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG12	8	0.54
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG13	8	0.54
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG21	8	0.54
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG22	8	0.54
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG23	8	0.54
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	2	0.54
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	2	0.54
(1,71)	1:23:A:PRO:HA	1:23:A:PRO:HB2	8	0.54
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD2	1	0.54
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD3	1	0.54
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD2	5	0.54
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD3	5	0.54
(1,5)	1:4:A:ALA:H	1:4:A:ALA:HA	9	0.54
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.53
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.53
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.53
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.53
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.53
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.53
(1,270)	1:19:A:SER:H	1:19:A:SER:HB3	7	0.53
(1,247)	1:21:A:ARG:H	1:21:A:ARG:HG2	8	0.53
(1,231)	1:11:A:TRP:HB3	1:12:A:LEU:H	7	0.53
(1,193)	1:20:A:GLY:H	1:20:A:GLY:HA2	4	0.53
(1,165)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.53
(1,141)	1:7:A:LEU:H	1:8:A:TYR:H	5	0.53
(1,117)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	2	0.53
(1,103)	1:10:A:GLN:H	1:10:A:GLN:HG2	4	0.53
(1,87)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	2	0.53
(1,87)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	3	0.53
(1,87)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	8	0.53
(1,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	9	0.53
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD2	4	0.53
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD3	4	0.53
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD2	8	0.53
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD3	8	0.53
(1,24)	1:25:A:SER:H	1:25:A:SER:HB2	10	0.53
(1,24)	1:25:A:SER:H	1:25:A:SER:HB3	10	0.53
(1,5)	1:4:A:ALA:H	1:4:A:ALA:HA	4	0.53
(3,159)	1:7:A:LEU:H	1:7:A:LEU:HB2	7	0.52
(2,166)	1:7:A:LEU:H	1:7:A:LEU:HB2	7	0.52
(1,334)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	1	0.52
(1,334)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	1	0.52
(1,334)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	1	0.52
(1,334)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	1	0.52
(1,334)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	1	0.52
(1,334)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	1	0.52
(1,281)	1:11:A:TRP:HE3	1:12:A:LEU:H	4	0.52
(1,273)	1:13:A:LYS:H	1:14:A:GLN:H	8	0.52
(1,231)	1:11:A:TRP:HB3	1:12:A:LEU:H	5	0.52
(1,193)	1:20:A:GLY:H	1:20:A:GLY:HA2	1	0.52
(1,193)	1:20:A:GLY:H	1:20:A:GLY:HA2	3	0.52
(1,193)	1:20:A:GLY:H	1:20:A:GLY:HA2	6	0.52
(1,193)	1:20:A:GLY:H	1:20:A:GLY:HA2	7	0.52
(1,162)	1:7:A:LEU:HD21	1:7:A:LEU:HG	1	0.52
(1,162)	1:7:A:LEU:HD22	1:7:A:LEU:HG	1	0.52
(1,162)	1:7:A:LEU:HD23	1:7:A:LEU:HG	1	0.52
(1,162)	1:7:A:LEU:HD21	1:7:A:LEU:HG	3	0.52
(1,162)	1:7:A:LEU:HD22	1:7:A:LEU:HG	3	0.52
(1,162)	1:7:A:LEU:HD23	1:7:A:LEU:HG	3	0.52
(1,162)	1:7:A:LEU:HD21	1:7:A:LEU:HG	6	0.52
(1,162)	1:7:A:LEU:HD22	1:7:A:LEU:HG	6	0.52
(1,162)	1:7:A:LEU:HD23	1:7:A:LEU:HG	6	0.52
(1,162)	1:7:A:LEU:HD21	1:7:A:LEU:HG	10	0.52
(1,162)	1:7:A:LEU:HD22	1:7:A:LEU:HG	10	0.52
(1,162)	1:7:A:LEU:HD23	1:7:A:LEU:HG	10	0.52
(1,127)	1:14:A:GLN:H	1:14:A:GLN:HA	9	0.52
(1,127)	1:14:A:GLN:H	1:14:A:GLN:HA	10	0.52
(1,86)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.52
(1,71)	1:23:A:PRO:HA	1:23:A:PRO:HB2	3	0.52
(1,71)	1:23:A:PRO:HA	1:23:A:PRO:HB2	5	0.52
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD2	4	0.52
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD3	4	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	1	0.52
(1,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	3	0.52
(1,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	8	0.52
(1,5)	1:4:A:ALA:H	1:4:A:ALA:HA	1	0.52
(1,5)	1:4:A:ALA:H	1:4:A:ALA:HA	2	0.52
(1,5)	1:4:A:ALA:H	1:4:A:ALA:HA	5	0.52
(1,5)	1:4:A:ALA:H	1:4:A:ALA:HA	7	0.52
(1,5)	1:4:A:ALA:H	1:4:A:ALA:HA	8	0.52
(1,5)	1:4:A:ALA:H	1:4:A:ALA:HA	10	0.52
(1,329)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	10	0.51
(1,329)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	10	0.51
(1,329)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	10	0.51
(1,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	0.51
(1,286)	1:21:A:ARG:H	1:21:A:ARG:HB2	4	0.51
(1,273)	1:13:A:LYS:H	1:14:A:GLN:H	1	0.51
(1,273)	1:13:A:LYS:H	1:14:A:GLN:H	4	0.51
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	10	0.51
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	10	0.51
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	10	0.51
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	10	0.51
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	10	0.51
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	10	0.51
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	10	0.51
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	10	0.51
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	10	0.51
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	10	0.51
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	10	0.51
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	10	0.51
(1,231)	1:11:A:TRP:HB3	1:12:A:LEU:H	2	0.51
(1,223)	1:15:A:GLY:H	1:16:A:GLY:H	8	0.51
(1,193)	1:20:A:GLY:H	1:20:A:GLY:HA2	2	0.51
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.51
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.51
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.51
(1,149)	1:3:A:GLU:HA	1:3:A:GLU:HB3	5	0.51
(1,145)	1:5:A:VAL:HA	1:5:A:VAL:HB	6	0.51
(1,112)	1:6:A:ARG:HA	1:6:A:ARG:HB3	1	0.51
(1,112)	1:6:A:ARG:HA	1:6:A:ARG:HB3	9	0.51
(1,108)	1:6:A:ARG:H	1:6:A:ARG:HB2	2	0.51
(1,98)	1:10:A:GLN:HA	1:10:A:GLN:HG2	1	0.51
(1,86)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	1	0.51
(1,86)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	6	0.51
(1,86)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	8	0.51
(1,86)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	9	0.51
(1,71)	1:23:A:PRO:HA	1:23:A:PRO:HB2	1	0.51
(1,71)	1:23:A:PRO:HA	1:23:A:PRO:HB2	2	0.51
(1,71)	1:23:A:PRO:HA	1:23:A:PRO:HB2	7	0.51
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD2	9	0.51
(1,65)	1:22:A:PRO:HA	1:23:A:PRO:HD3	9	0.51
(1,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	2	0.51
(1,44)	1:21:A:ARG:HA	1:21:A:ARG:HB3	4	0.51
(1,5)	1:4:A:ALA:H	1:4:A:ALA:HA	6	0.51
(1,280)	1:4:A:ALA:H	1:5:A:VAL:H	1	0.5
(1,246)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.5
(1,238)	1:3:A:GLU:H	1:3:A:GLU:HB2	10	0.5
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	8	0.5
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	8	0.5
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	8	0.5
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	8	0.5
(1,193)	1:20:A:GLY:H	1:20:A:GLY:HA2	9	0.5
(1,165)	1:7:A:LEU:H	1:7:A:LEU:HG	3	0.5
(1,162)	1:7:A:LEU:HD21	1:7:A:LEU:HG	5	0.5
(1,162)	1:7:A:LEU:HD22	1:7:A:LEU:HG	5	0.5
(1,162)	1:7:A:LEU:HD23	1:7:A:LEU:HG	5	0.5
(1,149)	1:3:A:GLU:HA	1:3:A:GLU:HB3	3	0.5
(1,103)	1:10:A:GLN:H	1:10:A:GLN:HG2	9	0.5
(1,98)	1:10:A:GLN:HA	1:10:A:GLN:HG2	8	0.5
(1,87)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	1	0.5
(1,87)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	10	0.5
(1,86)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	5	0.5
(1,71)	1:23:A:PRO:HA	1:23:A:PRO:HB2	9	0.5
(1,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.5
(1,44)	1:21:A:ARG:HA	1:21:A:ARG:HB3	8	0.5
(1,20)	1:2:A:GLU:HA	1:3:A:GLU:H	9	0.5
(1,5)	1:4:A:ALA:H	1:4:A:ALA:HA	3	0.5
(1,4)	1:3:A:GLU:H	1:3:A:GLU:HA	1	0.5
(3,299)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	1	0.49
(3,232)	1:6:A:ARG:HB3	1:7:A:LEU:H	3	0.49
(2,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	1	0.49
(2,242)	1:6:A:ARG:HB3	1:7:A:LEU:H	3	0.49
(1,304)	1:3:A:GLU:HA	1:6:A:ARG:HB3	10	0.49
(1,284)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	9	0.49
(1,260)	1:4:A:ALA:HB1	1:5:A:VAL:H	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,260)	1:4:A:ALA:HB2	1:5:A:VAL:H	5	0.49
(1,260)	1:4:A:ALA:HB3	1:5:A:VAL:H	5	0.49
(1,231)	1:11:A:TRP:HB3	1:12:A:LEU:H	9	0.49
(1,198)	1:12:A:LEU:HA	1:12:A:LEU:HB3	4	0.49
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	6	0.49
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	6	0.49
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	6	0.49
(1,162)	1:7:A:LEU:HD21	1:7:A:LEU:HG	9	0.49
(1,162)	1:7:A:LEU:HD22	1:7:A:LEU:HG	9	0.49
(1,162)	1:7:A:LEU:HD23	1:7:A:LEU:HG	9	0.49
(1,149)	1:3:A:GLU:HA	1:3:A:GLU:HB3	7	0.49
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG2	1	0.49
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG3	1	0.49
(1,112)	1:6:A:ARG:HA	1:6:A:ARG:HB3	5	0.49
(1,72)	1:23:A:PRO:HA	1:23:A:PRO:HG3	4	0.49
(1,71)	1:23:A:PRO:HA	1:23:A:PRO:HB2	10	0.49
(4,15)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	2	0.48
(3,280)	1:8:A:TYR:HA	1:11:A:TRP:HB2	10	0.48
(3,161)	1:7:A:LEU:H	1:7:A:LEU:HD11	2	0.48
(3,161)	1:7:A:LEU:H	1:7:A:LEU:HD12	2	0.48
(3,161)	1:7:A:LEU:H	1:7:A:LEU:HD13	2	0.48
(3,159)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.48
(3,130)	1:14:A:GLN:H	1:14:A:GLN:HG2	8	0.48
(2,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	2	0.48
(2,293)	1:8:A:TYR:HA	1:11:A:TRP:HB2	10	0.48
(2,168)	1:7:A:LEU:H	1:7:A:LEU:HD11	2	0.48
(2,168)	1:7:A:LEU:H	1:7:A:LEU:HD12	2	0.48
(2,168)	1:7:A:LEU:H	1:7:A:LEU:HD13	2	0.48
(2,166)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.48
(2,135)	1:14:A:GLN:H	1:14:A:GLN:HG2	8	0.48
(1,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	10	0.48
(1,260)	1:4:A:ALA:HB1	1:5:A:VAL:H	9	0.48
(1,260)	1:4:A:ALA:HB2	1:5:A:VAL:H	9	0.48
(1,260)	1:4:A:ALA:HB3	1:5:A:VAL:H	9	0.48
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	9	0.48
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	9	0.48
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	9	0.48
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	9	0.48
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	9	0.48
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	9	0.48
(1,223)	1:15:A:GLY:H	1:16:A:GLY:H	1	0.48
(1,223)	1:15:A:GLY:H	1:16:A:GLY:H	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,198)	1:12:A:LEU:HA	1:12:A:LEU:HB3	9	0.48
(1,177)	1:9:A:ILE:H	1:9:A:ILE:HG13	5	0.48
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	8	0.48
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	8	0.48
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	8	0.48
(1,162)	1:7:A:LEU:HD21	1:7:A:LEU:HG	4	0.48
(1,162)	1:7:A:LEU:HD22	1:7:A:LEU:HG	4	0.48
(1,162)	1:7:A:LEU:HD23	1:7:A:LEU:HG	4	0.48
(1,162)	1:7:A:LEU:HD21	1:7:A:LEU:HG	8	0.48
(1,162)	1:7:A:LEU:HD22	1:7:A:LEU:HG	8	0.48
(1,162)	1:7:A:LEU:HD23	1:7:A:LEU:HG	8	0.48
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG11	7	0.48
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG12	7	0.48
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG13	7	0.48
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG21	7	0.48
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG22	7	0.48
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG23	7	0.48
(1,87)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	6	0.48
(1,86)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	2	0.48
(1,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	7	0.48
(1,7)	1:3:A:GLU:HA	1:4:A:ALA:H	1	0.48
(1,4)	1:3:A:GLU:H	1:3:A:GLU:HA	2	0.48
(1,4)	1:3:A:GLU:H	1:3:A:GLU:HA	3	0.48
(3,317)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	1	0.47
(3,317)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	1	0.47
(3,317)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	1	0.47
(3,280)	1:8:A:TYR:HA	1:11:A:TRP:HB2	8	0.47
(3,159)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.47
(2,332)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	1	0.47
(2,332)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	1	0.47
(2,332)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	1	0.47
(2,293)	1:8:A:TYR:HA	1:11:A:TRP:HB2	8	0.47
(2,166)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.47
(1,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	8	0.47
(1,290)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	4	0.47
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	3	0.47
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	3	0.47
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	3	0.47
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	3	0.47
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	3	0.47
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	3	0.47
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	1	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	1	0.47
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	1	0.47
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	1	0.47
(1,198)	1:12:A:LEU:HA	1:12:A:LEU:HB3	1	0.47
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	3	0.47
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	3	0.47
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	3	0.47
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.47
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.47
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.47
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	4	0.47
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	4	0.47
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	4	0.47
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB2	10	0.47
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB3	10	0.47
(1,119)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	2	0.47
(1,87)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	9	0.47
(1,4)	1:3:A:GLU:H	1:3:A:GLU:HA	8	0.47
(3,317)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	3	0.46
(3,317)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	3	0.46
(3,317)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	3	0.46
(3,159)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.46
(2,332)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	3	0.46
(2,332)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	3	0.46
(2,332)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	3	0.46
(2,166)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.46
(1,297)	1:8:A:TYR:HA	1:11:A:TRP:HB3	4	0.46
(1,267)	1:18:A:SER:H	1:18:A:SER:HB2	8	0.46
(1,267)	1:18:A:SER:H	1:18:A:SER:HB3	8	0.46
(1,239)	1:3:A:GLU:HB3	1:4:A:ALA:H	1	0.46
(1,198)	1:12:A:LEU:HA	1:12:A:LEU:HB3	10	0.46
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB2	4	0.46
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB3	4	0.46
(1,135)	1:14:A:GLN:H	1:14:A:GLN:HG2	5	0.46
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB2	6	0.46
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB3	6	0.46
(1,98)	1:10:A:GLN:HA	1:10:A:GLN:HG2	5	0.46
(1,98)	1:10:A:GLN:HA	1:10:A:GLN:HG2	6	0.46
(1,87)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	5	0.46
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	6	0.46
(1,69)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	6	0.46
(1,20)	1:2:A:GLU:HA	1:3:A:GLU:H	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	3	0.45
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	3	0.45
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	3	0.45
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	3	0.45
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	3	0.45
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	3	0.45
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	3	0.45
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	3	0.45
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	3	0.45
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	3	0.45
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	3	0.45
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	3	0.45
(1,286)	1:21:A:ARG:H	1:21:A:ARG:HB2	8	0.45
(1,281)	1:11:A:TRP:HE3	1:12:A:LEU:H	5	0.45
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	8	0.45
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	8	0.45
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	8	0.45
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	8	0.45
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	8	0.45
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	8	0.45
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	4	0.45
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	4	0.45
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	4	0.45
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	4	0.45
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	4	0.45
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	4	0.45
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	4	0.45
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	4	0.45
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	4	0.45
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	4	0.45
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	4	0.45
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	4	0.45
(1,198)	1:12:A:LEU:HA	1:12:A:LEU:HB3	3	0.45
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	9	0.45
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	9	0.45
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	9	0.45
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	5	0.45
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	5	0.45
(1,44)	1:21:A:ARG:HA	1:21:A:ARG:HB3	2	0.45
(1,44)	1:21:A:ARG:HA	1:21:A:ARG:HB3	3	0.45
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG2	10	0.45
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG3	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,280)	1:8:A:TYR:HA	1:11:A:TRP:HB2	1	0.44
(3,280)	1:8:A:TYR:HA	1:11:A:TRP:HB2	5	0.44
(3,280)	1:8:A:TYR:HA	1:11:A:TRP:HB2	6	0.44
(2,293)	1:8:A:TYR:HA	1:11:A:TRP:HB2	1	0.44
(2,293)	1:8:A:TYR:HA	1:11:A:TRP:HB2	5	0.44
(2,293)	1:8:A:TYR:HA	1:11:A:TRP:HB2	6	0.44
(1,294)	1:8:A:TYR:HA	1:24:A:PRO:HD2	8	0.44
(1,290)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	2	0.44
(1,290)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	9	0.44
(1,279)	1:19:A:SER:H	1:20:A:GLY:H	5	0.44
(1,239)	1:3:A:GLU:HB3	1:4:A:ALA:H	8	0.44
(1,231)	1:11:A:TRP:HB3	1:12:A:LEU:H	4	0.44
(1,198)	1:12:A:LEU:HA	1:12:A:LEU:HB3	5	0.44
(1,198)	1:12:A:LEU:HA	1:12:A:LEU:HB3	6	0.44
(1,198)	1:12:A:LEU:HA	1:12:A:LEU:HB3	7	0.44
(1,157)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	4	0.44
(1,157)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	8	0.44
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.44
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.44
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.44
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.44
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.44
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.44
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	0.44
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	0.44
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	0.44
(1,149)	1:3:A:GLU:HA	1:3:A:GLU:HB3	9	0.44
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB2	2	0.44
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB3	2	0.44
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB2	3	0.44
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB3	3	0.44
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB2	7	0.44
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB3	7	0.44
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB2	9	0.44
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB3	9	0.44
(1,121)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	3	0.44
(1,113)	1:6:A:ARG:HA	1:6:A:ARG:HB2	5	0.44
(1,112)	1:6:A:ARG:HA	1:6:A:ARG:HB3	3	0.44
(1,108)	1:6:A:ARG:H	1:6:A:ARG:HB2	4	0.44
(1,86)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	4	0.44
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	6	0.44
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:3:A:GLU:H	1:3:A:GLU:HA	5	0.44
(1,4)	1:3:A:GLU:H	1:3:A:GLU:HA	9	0.44
(1,4)	1:3:A:GLU:H	1:3:A:GLU:HA	10	0.44
(4,15)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	1	0.43
(3,309)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	4	0.43
(3,309)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	4	0.43
(3,309)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	4	0.43
(3,297)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	7	0.43
(3,280)	1:8:A:TYR:HA	1:11:A:TRP:HB2	7	0.43
(3,159)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.43
(2,324)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	4	0.43
(2,324)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	4	0.43
(2,324)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	4	0.43
(2,312)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	7	0.43
(2,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	1	0.43
(2,293)	1:8:A:TYR:HA	1:11:A:TRP:HB2	7	0.43
(2,166)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.43
(1,290)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	5	0.43
(1,290)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	7	0.43
(1,269)	1:19:A:SER:H	1:19:A:SER:HB2	6	0.43
(1,255)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	9	0.43
(1,255)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	9	0.43
(1,198)	1:12:A:LEU:HA	1:12:A:LEU:HB3	8	0.43
(1,157)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	5	0.43
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.43
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.43
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.43
(1,149)	1:3:A:GLU:HA	1:3:A:GLU:HB3	1	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG11	3	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG12	3	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG13	3	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG21	3	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG22	3	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG23	3	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG11	9	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG12	9	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG13	9	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG21	9	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG22	9	0.43
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG23	9	0.43
(1,140)	1:11:A:TRP:H	1:12:A:LEU:H	9	0.43
(1,121)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:6:A:ARG:HA	1:6:A:ARG:HB2	3	0.43
(1,64)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	1	0.43
(1,64)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	2	0.43
(1,64)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	3	0.43
(1,64)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	4	0.43
(1,64)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	5	0.43
(1,64)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	6	0.43
(1,64)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	7	0.43
(1,64)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	8	0.43
(1,64)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	9	0.43
(1,64)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.43
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	5	0.43
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	5	0.43
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD2	7	0.43
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD3	7	0.43
(1,23)	1:25:A:SER:H	1:25:A:SER:HA	9	0.43
(4,15)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	4	0.42
(2,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	4	0.42
(1,286)	1:21:A:ARG:H	1:21:A:ARG:HB2	5	0.42
(1,284)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	4	0.42
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	2	0.42
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	2	0.42
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	2	0.42
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	2	0.42
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	2	0.42
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	2	0.42
(1,198)	1:12:A:LEU:HA	1:12:A:LEU:HB3	2	0.42
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	8	0.42
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	8	0.42
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	8	0.42
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	8	0.42
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	8	0.42
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	8	0.42
(1,157)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	1	0.42
(1,157)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	2	0.42
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.42
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.42
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.42
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG11	4	0.42
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG12	4	0.42
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG13	4	0.42
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG21	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG22	4	0.42
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG23	4	0.42
(1,110)	1:6:A:ARG:H	1:6:A:ARG:HG3	10	0.42
(1,87)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	4	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	1	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	1	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	2	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	2	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	3	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	3	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	4	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	4	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	7	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	7	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	8	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	8	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	9	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	9	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.42
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	10	0.42
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	8	0.42
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	8	0.42
(1,24)	1:25:A:SER:H	1:25:A:SER:HB2	4	0.42
(1,24)	1:25:A:SER:H	1:25:A:SER:HB3	4	0.42
(1,7)	1:3:A:GLU:HA	1:4:A:ALA:H	2	0.42
(4,8)	1:7:A:LEU:H	1:8:A:TYR:HB3	9	0.41
(4,1)	1:17:A:PRO:HA	1:17:A:PRO:HD2	4	0.41
(3,296)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	6	0.41
(3,280)	1:8:A:TYR:HA	1:11:A:TRP:HB2	4	0.41
(3,235)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.41
(3,103)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.41
(2,310)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	6	0.41
(2,293)	1:8:A:TYR:HA	1:11:A:TRP:HB2	4	0.41
(2,246)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.41
(2,232)	1:7:A:LEU:H	1:8:A:TYR:HB3	9	0.41
(2,108)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.41
(2,28)	1:17:A:PRO:HA	1:17:A:PRO:HD2	4	0.41
(1,335)	1:7:A:LEU:HD11	1:8:A:TYR:HB2	8	0.41
(1,335)	1:7:A:LEU:HD12	1:8:A:TYR:HB2	8	0.41
(1,335)	1:7:A:LEU:HD13	1:8:A:TYR:HB2	8	0.41
(1,321)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	9	0.41
(1,260)	1:4:A:ALA:HB1	1:5:A:VAL:H	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,260)	1:4:A:ALA:HB2	1:5:A:VAL:H	8	0.41
(1,260)	1:4:A:ALA:HB3	1:5:A:VAL:H	8	0.41
(1,223)	1:15:A:GLY:H	1:16:A:GLY:H	5	0.41
(1,157)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	3	0.41
(1,157)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	7	0.41
(1,157)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	9	0.41
(1,157)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.41
(1,148)	1:3:A:GLU:HA	1:3:A:GLU:HB2	4	0.41
(1,141)	1:7:A:LEU:H	1:8:A:TYR:H	9	0.41
(1,140)	1:11:A:TRP:H	1:12:A:LEU:H	10	0.41
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB2	8	0.41
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB3	8	0.41
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB2	4	0.41
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB3	4	0.41
(1,115)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	3	0.41
(1,74)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	1	0.41
(1,74)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	2	0.41
(1,74)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	5	0.41
(1,74)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	6	0.41
(1,74)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	8	0.41
(1,74)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	9	0.41
(1,74)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	1	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	1	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	2	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	2	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	3	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	3	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	4	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	4	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	7	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	7	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	9	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	9	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	10	0.41
(1,58)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.41
(1,7)	1:3:A:GLU:HA	1:4:A:ALA:H	3	0.41
(1,4)	1:3:A:GLU:H	1:3:A:GLU:HA	6	0.41
(1,4)	1:3:A:GLU:H	1:3:A:GLU:HA	7	0.41
(4,1)	1:17:A:PRO:HA	1:17:A:PRO:HD2	2	0.4
(4,1)	1:17:A:PRO:HA	1:17:A:PRO:HD2	7	0.4
(3,309)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,309)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	2	0.4
(3,309)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	2	0.4
(3,195)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	4	0.4
(3,195)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	4	0.4
(3,195)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	4	0.4
(2,324)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	2	0.4
(2,324)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	2	0.4
(2,324)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	2	0.4
(2,202)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	4	0.4
(2,202)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	4	0.4
(2,202)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	4	0.4
(2,28)	1:17:A:PRO:HA	1:17:A:PRO:HD2	2	0.4
(2,28)	1:17:A:PRO:HA	1:17:A:PRO:HD2	7	0.4
(1,305)	1:6:A:ARG:HA	1:9:A:ILE:HB	9	0.4
(1,304)	1:3:A:GLU:HA	1:6:A:ARG:HB3	4	0.4
(1,290)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	8	0.4
(1,281)	1:11:A:TRP:HE3	1:12:A:LEU:H	8	0.4
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	5	0.4
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	5	0.4
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	5	0.4
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	5	0.4
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	5	0.4
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	5	0.4
(1,247)	1:21:A:ARG:H	1:21:A:ARG:HG2	1	0.4
(1,208)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	4	0.4
(1,208)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	4	0.4
(1,208)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	4	0.4
(1,157)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	6	0.4
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB2	2	0.4
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB3	2	0.4
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB2	8	0.4
(1,128)	1:14:A:GLN:HA	1:14:A:GLN:HB3	8	0.4
(1,117)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	6	0.4
(1,113)	1:6:A:ARG:HA	1:6:A:ARG:HB2	9	0.4
(1,74)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	3	0.4
(1,74)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	7	0.4
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG2	6	0.4
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG3	6	0.4
(4,1)	1:17:A:PRO:HA	1:17:A:PRO:HD2	1	0.39
(4,1)	1:17:A:PRO:HA	1:17:A:PRO:HD2	3	0.39
(4,1)	1:17:A:PRO:HA	1:17:A:PRO:HD2	9	0.39
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	4	0.39
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	4	0.39
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	4	0.39
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	4	0.39
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	4	0.39
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	6	0.39
(3,244)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	6	0.39
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	6	0.39
(3,244)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	6	0.39
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	6	0.39
(3,244)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	6	0.39
(3,103)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.39
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	4	0.39
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	4	0.39
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	4	0.39
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	4	0.39
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	4	0.39
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	4	0.39
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	6	0.39
(2,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	6	0.39
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	6	0.39
(2,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	6	0.39
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	6	0.39
(2,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	6	0.39
(2,108)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.39
(2,28)	1:17:A:PRO:HA	1:17:A:PRO:HD2	1	0.39
(2,28)	1:17:A:PRO:HA	1:17:A:PRO:HD2	3	0.39
(2,28)	1:17:A:PRO:HA	1:17:A:PRO:HD2	9	0.39
(1,315)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	6	0.39
(1,313)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	8	0.39
(1,284)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	10	0.39
(1,281)	1:11:A:TRP:HE3	1:12:A:LEU:H	10	0.39
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	4	0.39
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	4	0.39
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	4	0.39
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	4	0.39
(1,177)	1:9:A:ILE:H	1:9:A:ILE:HG13	7	0.39
(1,153)	1:7:A:LEU:HA	1:7:A:LEU:HG	5	0.39
(1,141)	1:7:A:LEU:H	1:8:A:TYR:H	3	0.39
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB2	3	0.39
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB3	3	0.39
(1,115)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:22:A:PRO:HA	1:22:A:PRO:HD2	6	0.39
(1,44)	1:21:A:ARG:HA	1:21:A:ARG:HB3	9	0.39
(1,23)	1:25:A:SER:H	1:25:A:SER:HA	4	0.39
(4,15)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	9	0.38
(2,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	9	0.38
(1,290)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	1	0.38
(1,290)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	6	0.38
(1,290)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	10	0.38
(1,281)	1:11:A:TRP:HE3	1:12:A:LEU:H	2	0.38
(1,270)	1:19:A:SER:H	1:19:A:SER:HB3	8	0.38
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	7	0.38
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	7	0.38
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	7	0.38
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	7	0.38
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	7	0.38
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	7	0.38
(1,223)	1:15:A:GLY:H	1:16:A:GLY:H	7	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	1	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	1	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	1	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	1	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	2	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	2	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	2	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	2	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	3	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	3	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	3	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	3	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	5	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	5	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	5	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	5	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	6	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	6	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	6	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	6	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	7	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	7	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	7	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	7	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	8	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	8	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	8	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	9	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	9	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	9	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	9	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	10	0.38
(1,217)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	10	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	10	0.38
(1,217)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	10	0.38
(1,148)	1:3:A:GLU:HA	1:3:A:GLU:HB2	6	0.38
(1,141)	1:7:A:LEU:H	1:8:A:TYR:H	1	0.38
(1,141)	1:7:A:LEU:H	1:8:A:TYR:H	10	0.38
(1,115)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	1	0.38
(1,113)	1:6:A:ARG:HA	1:6:A:ARG:HB2	1	0.38
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG2	8	0.38
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG3	8	0.38
(1,23)	1:25:A:SER:H	1:25:A:SER:HA	1	0.38
(1,23)	1:25:A:SER:H	1:25:A:SER:HA	5	0.38
(1,23)	1:25:A:SER:H	1:25:A:SER:HA	10	0.38
(1,4)	1:3:A:GLU:H	1:3:A:GLU:HA	4	0.38
(4,8)	1:7:A:LEU:H	1:8:A:TYR:HB3	3	0.37
(4,8)	1:7:A:LEU:H	1:8:A:TYR:HB3	10	0.37
(4,1)	1:17:A:PRO:HA	1:17:A:PRO:HD2	5	0.37
(3,286)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	4	0.37
(3,103)	1:6:A:ARG:H	1:6:A:ARG:HB2	9	0.37
(2,299)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	4	0.37
(2,232)	1:7:A:LEU:H	1:8:A:TYR:HB3	3	0.37
(2,232)	1:7:A:LEU:H	1:8:A:TYR:HB3	10	0.37
(2,108)	1:6:A:ARG:H	1:6:A:ARG:HB2	9	0.37
(2,28)	1:17:A:PRO:HA	1:17:A:PRO:HD2	5	0.37
(1,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	1	0.37
(1,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	1	0.37
(1,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	1	0.37
(1,327)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	0.37
(1,327)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	0.37
(1,327)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	0.37
(1,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	3	0.37
(1,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	3	0.37
(1,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	3	0.37
(1,327)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	3	0.37
(1,327)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	3	0.37
(1,301)	1:8:A:TYR:HB2	1:24:A:PRO:HD2	4	0.37
(1,296)	1:8:A:TYR:HA	1:24:A:PRO:HD3	5	0.37
(1,290)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	3	0.37
(1,281)	1:11:A:TRP:HE3	1:12:A:LEU:H	7	0.37
(1,275)	1:9:A:ILE:H	1:10:A:GLN:H	4	0.37
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	6	0.37
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	6	0.37
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	6	0.37
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	6	0.37
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	6	0.37
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	6	0.37
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	10	0.37
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	10	0.37
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	10	0.37
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	10	0.37
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	10	0.37
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	10	0.37
(1,244)	1:12:A:LEU:HB2	1:13:A:LYS:H	4	0.37
(1,238)	1:3:A:GLU:H	1:3:A:GLU:HB2	1	0.37
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	7	0.37
(1,213)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	7	0.37
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	7	0.37
(1,213)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	7	0.37
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG11	6	0.37
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG12	6	0.37
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG13	6	0.37
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG21	6	0.37
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG22	6	0.37
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG23	6	0.37
(1,114)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	10	0.37
(1,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	8	0.37
(1,74)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	4	0.37
(1,47)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	1	0.37
(1,47)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	2	0.37
(1,47)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	8	0.37
(1,47)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	9	0.37
(4,8)	1:7:A:LEU:H	1:8:A:TYR:HB3	1	0.36
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD21	3	0.36
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD22	3	0.36
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD23	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.36
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.36
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.36
(3,103)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	0.36
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD21	3	0.36
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD22	3	0.36
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD23	3	0.36
(2,232)	1:7:A:LEU:H	1:8:A:TYR:HB3	1	0.36
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.36
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.36
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.36
(2,108)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	0.36
(1,297)	1:8:A:TYR:HA	1:11:A:TRP:HB3	2	0.36
(1,238)	1:3:A:GLU:H	1:3:A:GLU:HB2	7	0.36
(1,223)	1:15:A:GLY:H	1:16:A:GLY:H	3	0.36
(1,148)	1:3:A:GLU:HA	1:3:A:GLU:HB2	10	0.36
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB2	7	0.36
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB3	7	0.36
(1,130)	1:14:A:GLN:HA	1:14:A:GLN:HG3	8	0.36
(1,122)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	3	0.36
(1,122)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	7	0.36
(1,118)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	2	0.36
(1,86)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	7	0.36
(1,47)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	3	0.36
(1,47)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	4	0.36
(1,47)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	5	0.36
(1,47)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	6	0.36
(1,47)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	10	0.36
(1,44)	1:21:A:ARG:HA	1:21:A:ARG:HB3	5	0.36
(1,23)	1:25:A:SER:H	1:25:A:SER:HA	6	0.36
(1,23)	1:25:A:SER:H	1:25:A:SER:HA	7	0.36
(1,23)	1:25:A:SER:H	1:25:A:SER:HA	8	0.36
(1,7)	1:3:A:GLU:HA	1:4:A:ALA:H	4	0.36
(4,1)	1:17:A:PRO:HA	1:17:A:PRO:HD2	6	0.35
(3,236)	1:21:A:ARG:H	1:21:A:ARG:HG2	7	0.35
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.35
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.35
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.35
(2,247)	1:21:A:ARG:H	1:21:A:ARG:HG2	7	0.35
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.35
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.35
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,28)	1:17:A:PRO:HA	1:17:A:PRO:HD2	6	0.35
(1,291)	1:21:A:ARG:HA	1:22:A:PRO:HD2	6	0.35
(1,275)	1:9:A:ILE:H	1:10:A:GLN:H	9	0.35
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	1	0.35
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	1	0.35
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	1	0.35
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	1	0.35
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	1	0.35
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	1	0.35
(1,255)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	4	0.35
(1,255)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	4	0.35
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB2	2	0.35
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB2	3	0.35
(1,185)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	2	0.35
(1,185)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	2	0.35
(1,185)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	2	0.35
(1,185)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	7	0.35
(1,185)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	7	0.35
(1,185)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	7	0.35
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	4	0.35
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	4	0.35
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	4	0.35
(1,148)	1:3:A:GLU:HA	1:3:A:GLU:HB2	8	0.35
(1,139)	1:5:A:VAL:H	1:6:A:ARG:H	5	0.35
(1,122)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	2	0.35
(1,122)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	4	0.35
(1,122)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	6	0.35
(1,122)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	8	0.35
(1,122)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.35
(1,109)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.35
(1,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	4	0.35
(1,47)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	7	0.35
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	7	0.35
(1,43)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	7	0.35
(1,23)	1:25:A:SER:H	1:25:A:SER:HA	2	0.35
(1,23)	1:25:A:SER:H	1:25:A:SER:HA	3	0.35
(4,15)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	3	0.34
(4,14)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	4	0.34
(3,247)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	9	0.34
(3,247)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	9	0.34
(3,245)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	4	0.34
(3,245)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,245)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	4	0.34
(3,245)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	4	0.34
(3,245)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	4	0.34
(3,245)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	4	0.34
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.34
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.34
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.34
(2,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	3	0.34
(2,302)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	4	0.34
(2,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	9	0.34
(2,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	9	0.34
(2,257)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	4	0.34
(2,257)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	4	0.34
(2,257)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	4	0.34
(2,257)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	4	0.34
(2,257)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	4	0.34
(2,257)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	4	0.34
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.34
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.34
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.34
(1,245)	1:7:A:LEU:HB2	1:8:A:TYR:H	5	0.34
(1,185)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	5	0.34
(1,185)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	5	0.34
(1,185)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	5	0.34
(1,185)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	9	0.34
(1,185)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	9	0.34
(1,185)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	9	0.34
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	3	0.34
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	3	0.34
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	3	0.34
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	10	0.34
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	10	0.34
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	10	0.34
(1,140)	1:11:A:TRP:H	1:12:A:LEU:H	1	0.34
(1,134)	1:14:A:GLN:H	1:14:A:GLN:HG3	8	0.34
(1,123)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	6	0.34
(1,122)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	1	0.34
(1,122)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	5	0.34
(1,122)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	9	0.34
(1,118)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	3	0.34
(1,115)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	9	0.34
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	6	0.34
(1,46)	1:21:A:ARG:HA	1:21:A:ARG:HG2	6	0.34
(1,46)	1:21:A:ARG:HA	1:21:A:ARG:HG3	6	0.34
(4,8)	1:7:A:LEU:H	1:8:A:TYR:HB3	5	0.33
(4,1)	1:17:A:PRO:HA	1:17:A:PRO:HD2	8	0.33
(3,309)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	8	0.33
(3,309)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	8	0.33
(3,309)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	8	0.33
(3,247)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	4	0.33
(3,247)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	4	0.33
(2,324)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	8	0.33
(2,324)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	8	0.33
(2,324)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	8	0.33
(2,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	4	0.33
(2,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	4	0.33
(2,232)	1:7:A:LEU:H	1:8:A:TYR:HB3	5	0.33
(2,28)	1:17:A:PRO:HA	1:17:A:PRO:HD2	8	0.33
(1,330)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	3	0.33
(1,330)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	3	0.33
(1,330)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	3	0.33
(1,279)	1:19:A:SER:H	1:20:A:GLY:H	10	0.33
(1,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	7	0.33
(1,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	7	0.33
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB2	3	0.33
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB3	3	0.33
(1,185)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	1	0.33
(1,185)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	1	0.33
(1,185)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	1	0.33
(1,185)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	3	0.33
(1,185)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	3	0.33
(1,185)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	3	0.33
(1,185)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	4	0.33
(1,185)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	4	0.33
(1,185)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	4	0.33
(1,185)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	6	0.33
(1,185)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	6	0.33
(1,185)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	6	0.33
(1,185)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	8	0.33
(1,185)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	8	0.33
(1,185)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	8	0.33
(1,185)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	10	0.33
(1,185)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	10	0.33
(1,133)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	2	0.33
(1,133)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	2	0.33
(1,118)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	8	0.33
(1,71)	1:23:A:PRO:HA	1:23:A:PRO:HB2	6	0.33
(1,44)	1:21:A:ARG:HA	1:21:A:ARG:HB3	1	0.33
(3,318)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	4	0.32
(3,318)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	4	0.32
(3,318)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	4	0.32
(3,318)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	4	0.32
(3,318)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	4	0.32
(3,318)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	4	0.32
(3,237)	1:5:A:VAL:HB	1:6:A:ARG:H	5	0.32
(2,333)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	4	0.32
(2,333)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	4	0.32
(2,333)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	4	0.32
(2,333)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	4	0.32
(2,333)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	4	0.32
(2,333)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	4	0.32
(2,248)	1:5:A:VAL:HB	1:6:A:ARG:H	5	0.32
(1,326)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	3	0.32
(1,326)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	3	0.32
(1,326)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	3	0.32
(1,326)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	3	0.32
(1,326)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	3	0.32
(1,326)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	3	0.32
(1,326)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	7	0.32
(1,326)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	7	0.32
(1,326)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	7	0.32
(1,326)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	7	0.32
(1,326)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	7	0.32
(1,326)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	7	0.32
(1,284)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	2	0.32
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	1	0.32
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	1	0.32
(1,164)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	1	0.32
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	5	0.32
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	5	0.32
(1,161)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	5	0.32
(1,152)	1:7:A:LEU:HA	1:7:A:LEU:HB2	2	0.32
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG11	10	0.32
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG12	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG13	10	0.32
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.32
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.32
(1,144)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.32
(1,140)	1:11:A:TRP:H	1:12:A:LEU:H	3	0.32
(1,133)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	8	0.32
(1,133)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	8	0.32
(1,130)	1:14:A:GLN:HA	1:14:A:GLN:HG3	4	0.32
(1,118)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	1	0.32
(1,118)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	5	0.32
(1,118)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	7	0.32
(1,118)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	9	0.32
(1,113)	1:6:A:ARG:HA	1:6:A:ARG:HB2	4	0.32
(1,25)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	1	0.32
(1,25)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	2	0.32
(1,25)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	3	0.32
(1,25)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	4	0.32
(1,25)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	5	0.32
(1,25)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	6	0.32
(1,25)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	7	0.32
(1,25)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	8	0.32
(1,25)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	9	0.32
(1,25)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.32
(3,312)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	4	0.31
(3,312)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	4	0.31
(3,312)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	4	0.31
(3,280)	1:8:A:TYR:HA	1:11:A:TRP:HB2	9	0.31
(3,223)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.31
(2,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	4	0.31
(2,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	4	0.31
(2,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	4	0.31
(2,293)	1:8:A:TYR:HA	1:11:A:TRP:HB2	9	0.31
(2,230)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.31
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	2	0.31
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	2	0.31
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	2	0.31
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	2	0.31
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	2	0.31
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	2	0.31
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	2	0.31
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	2	0.31
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	2	0.31
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	2	0.31
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	2	0.31
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB2	6	0.31
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB2	9	0.31
(1,237)	1:3:A:GLU:H	1:3:A:GLU:HB3	9	0.31
(1,194)	1:20:A:GLY:H	1:20:A:GLY:HA3	10	0.31
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	6	0.31
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	6	0.31
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	6	0.31
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	5	0.31
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	5	0.31
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	5	0.31
(1,135)	1:14:A:GLN:H	1:14:A:GLN:HG2	3	0.31
(1,133)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	10	0.31
(1,133)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	10	0.31
(1,110)	1:6:A:ARG:H	1:6:A:ARG:HG3	7	0.31
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.3
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.3
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.3
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.3
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.3
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.3
(3,280)	1:8:A:TYR:HA	1:11:A:TRP:HB2	2	0.3
(3,235)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.3
(2,293)	1:8:A:TYR:HA	1:11:A:TRP:HB2	2	0.3
(2,246)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.3
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.3
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.3
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.3
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.3
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.3
(2,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.3
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG11	3	0.3
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG12	3	0.3
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG13	3	0.3
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG21	3	0.3
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG22	3	0.3
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG23	3	0.3
(1,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	10	0.3
(1,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	10	0.3
(1,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.3
(1,327)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.3
(1,327)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.3
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	10	0.3
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	10	0.3
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	10	0.3
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	10	0.3
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	10	0.3
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	10	0.3
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	10	0.3
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	10	0.3
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	10	0.3
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	10	0.3
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	10	0.3
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	10	0.3
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	10	0.3
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	10	0.3
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	10	0.3
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	10	0.3
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	10	0.3
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	10	0.3
(1,313)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	7	0.3
(1,296)	1:8:A:TYR:HA	1:24:A:PRO:HD3	9	0.3
(1,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	5	0.3
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB2	8	0.3
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	8	0.3
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	8	0.3
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	8	0.3
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	6	0.3
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	6	0.3
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	6	0.3
(1,149)	1:3:A:GLU:HA	1:3:A:GLU:HB3	2	0.3
(1,139)	1:5:A:VAL:H	1:6:A:ARG:H	7	0.3
(1,134)	1:14:A:GLN:H	1:14:A:GLN:HG3	9	0.3
(1,133)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	3	0.3
(1,133)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	3	0.3
(1,133)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	4	0.3
(1,133)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	4	0.3
(1,130)	1:14:A:GLN:HA	1:14:A:GLN:HG3	2	0.3
(1,121)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	2	0.3
(4,4)	1:24:A:PRO:HA	1:24:A:PRO:HD3	5	0.29
(3,280)	1:8:A:TYR:HA	1:11:A:TRP:HB2	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,223)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.29
(3,223)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.29
(3,223)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.29
(2,293)	1:8:A:TYR:HA	1:11:A:TRP:HB2	3	0.29
(2,230)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.29
(2,230)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.29
(2,230)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.29
(2,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	5	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG11	2	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG12	2	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG13	2	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG21	2	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG22	2	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG23	2	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG11	4	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG12	4	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG13	4	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG21	4	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG22	4	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG23	4	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG11	5	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG12	5	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG13	5	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG21	5	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG22	5	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG23	5	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG11	6	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG12	6	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG13	6	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG21	6	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG22	6	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG23	6	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG11	7	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG12	7	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG13	7	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG21	7	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG22	7	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG23	7	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG11	8	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG12	8	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG13	8	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG21	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG22	8	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG23	8	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG11	10	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG12	10	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG13	10	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG21	10	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG22	10	0.29
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG23	10	0.29
(1,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	6	0.29
(1,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	6	0.29
(1,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	6	0.29
(1,327)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	6	0.29
(1,327)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	6	0.29
(1,327)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	6	0.29
(1,317)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	4	0.29
(1,316)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	4	0.29
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB2	10	0.29
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB3	10	0.29
(1,297)	1:8:A:TYR:HA	1:11:A:TRP:HB3	5	0.29
(1,275)	1:9:A:ILE:H	1:10:A:GLN:H	3	0.29
(1,275)	1:9:A:ILE:H	1:10:A:GLN:H	5	0.29
(1,275)	1:9:A:ILE:H	1:10:A:GLN:H	10	0.29
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB2	1	0.29
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB3	1	0.29
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB2	7	0.29
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD2	5	0.29
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD3	5	0.29
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	4	0.29
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	4	0.29
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	4	0.29
(1,181)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	1	0.29
(1,181)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	3	0.29
(1,181)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	4	0.29
(1,181)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	6	0.29
(1,181)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	8	0.29
(1,181)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	10	0.29
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	8	0.29
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	8	0.29
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	8	0.29
(1,133)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	5	0.29
(1,133)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	5	0.29
(1,115)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:3:A:GLU:HA	1:4:A:ALA:H	5	0.29
(4,10)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.28
(3,223)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.28
(3,223)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.28
(3,223)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.28
(2,240)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.28
(2,230)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.28
(2,230)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.28
(2,230)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.28
(1,317)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	8	0.28
(1,316)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	1	0.28
(1,316)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	2	0.28
(1,316)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	3	0.28
(1,316)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	7	0.28
(1,316)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	8	0.28
(1,316)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	10	0.28
(1,275)	1:9:A:ILE:H	1:10:A:GLN:H	1	0.28
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB2	5	0.28
(1,238)	1:3:A:GLU:H	1:3:A:GLU:HB2	3	0.28
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	3	0.28
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	3	0.28
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	3	0.28
(1,181)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	2	0.28
(1,181)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	5	0.28
(1,181)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	7	0.28
(1,181)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	9	0.28
(1,177)	1:9:A:ILE:H	1:9:A:ILE:HG13	9	0.28
(1,150)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	5	0.28
(1,150)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	5	0.28
(1,140)	1:11:A:TRP:H	1:12:A:LEU:H	4	0.28
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB2	6	0.28
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB3	6	0.28
(1,133)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	6	0.28
(1,133)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	6	0.28
(1,133)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	7	0.28
(1,133)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	7	0.28
(1,133)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	9	0.28
(1,133)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	9	0.28
(1,131)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	1	0.28
(1,131)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	2	0.28
(1,131)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	3	0.28
(1,131)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	5	0.28
(1,131)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	6	0.28
(1,131)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	8	0.28
(1,131)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	10	0.28
(1,123)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	4	0.28
(1,2)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	5	0.28
(3,237)	1:5:A:VAL:HB	1:6:A:ARG:H	2	0.27
(3,237)	1:5:A:VAL:HB	1:6:A:ARG:H	3	0.27
(3,235)	1:21:A:ARG:H	1:21:A:ARG:HB3	8	0.27
(3,223)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.27
(3,223)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.27
(2,248)	1:5:A:VAL:HB	1:6:A:ARG:H	2	0.27
(2,248)	1:5:A:VAL:HB	1:6:A:ARG:H	3	0.27
(2,246)	1:21:A:ARG:H	1:21:A:ARG:HB3	8	0.27
(2,230)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.27
(2,230)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG11	1	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG12	1	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG13	1	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG21	1	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG22	1	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG23	1	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG11	9	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG12	9	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG13	9	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG21	9	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG22	9	0.27
(1,328)	1:5:A:VAL:HB	1:5:A:VAL:HG23	9	0.27
(1,316)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	5	0.27
(1,316)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	6	0.27
(1,316)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	9	0.27
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB2	6	0.27
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB3	6	0.27
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB2	1	0.27
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	4	0.27
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	4	0.27
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	4	0.27
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	4	0.27
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	5	0.27
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	5	0.27
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	5	0.27
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	6	0.27
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	6	0.27
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	6	0.27
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	6	0.27
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	10	0.27
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	10	0.27
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	10	0.27
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	10	0.27
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	1	0.27
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	1	0.27
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	1	0.27
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.27
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.27
(1,186)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.27
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	4	0.27
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	4	0.27
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	4	0.27
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	10	0.27
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	10	0.27
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	10	0.27
(1,171)	1:9:A:ILE:HA	1:9:A:ILE:HG12	1	0.27
(1,152)	1:7:A:LEU:HA	1:7:A:LEU:HB2	4	0.27
(1,150)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	3	0.27
(1,150)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	3	0.27
(1,140)	1:11:A:TRP:H	1:12:A:LEU:H	7	0.27
(1,133)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	1	0.27
(1,133)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	1	0.27
(1,131)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	7	0.27
(1,131)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	9	0.27
(1,80)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	8	0.27
(1,44)	1:21:A:ARG:HA	1:21:A:ARG:HB3	6	0.27
(1,7)	1:3:A:GLU:HA	1:4:A:ALA:H	9	0.27
(1,2)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	1	0.27
(1,2)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	2	0.27
(1,2)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	3	0.27
(1,2)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	4	0.27
(1,2)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	6	0.27
(1,2)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	7	0.27
(1,2)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	8	0.27
(1,2)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	9	0.27
(1,2)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	10	0.27
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.26
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.26
(3,289)	1:3:A:GLU:HA	1:6:A:ARG:HB2	5	0.26
(3,242)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	4	0.26
(3,242)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	4	0.26
(3,242)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	4	0.26
(3,237)	1:5:A:VAL:HB	1:6:A:ARG:H	6	0.26
(3,106)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.26
(3,106)	1:6:A:ARG:H	1:6:A:ARG:HG2	6	0.26
(2,303)	1:3:A:GLU:HA	1:6:A:ARG:HB2	5	0.26
(2,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	4	0.26
(2,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	4	0.26
(2,253)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	4	0.26
(2,248)	1:5:A:VAL:HB	1:6:A:ARG:H	6	0.26
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.26
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.26
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.26
(2,111)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.26
(2,111)	1:6:A:ARG:H	1:6:A:ARG:HG2	6	0.26
(1,340)	1:4:A:ALA:HA	1:7:A:LEU:HD21	2	0.26
(1,340)	1:4:A:ALA:HA	1:7:A:LEU:HD22	2	0.26
(1,340)	1:4:A:ALA:HA	1:7:A:LEU:HD23	2	0.26
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	3	0.26
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	3	0.26
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	3	0.26
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	3	0.26
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	3	0.26
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	3	0.26
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	3	0.26
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	3	0.26
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	3	0.26
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	3	0.26
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	3	0.26
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	3	0.26
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	3	0.26
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	3	0.26
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	3	0.26
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	3	0.26
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	3	0.26
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	3	0.26
(1,255)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	10	0.26
(1,255)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB2	7	0.26
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB3	7	0.26
(1,235)	1:12:A:LEU:HA	1:16:A:GLY:H	3	0.26
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	2	0.26
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	2	0.26
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	2	0.26
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	2	0.26
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD2	4	0.26
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD3	4	0.26
(1,197)	1:12:A:LEU:HA	1:12:A:LEU:HB2	2	0.26
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	3	0.26
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	3	0.26
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	3	0.26
(1,111)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.26
(4,8)	1:7:A:LEU:H	1:8:A:TYR:HB3	6	0.25
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.25
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.25
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.25
(4,1)	1:17:A:PRO:HA	1:17:A:PRO:HD2	10	0.25
(3,289)	1:3:A:GLU:HA	1:6:A:ARG:HB2	1	0.25
(3,237)	1:5:A:VAL:HB	1:6:A:ARG:H	7	0.25
(3,89)	1:24:A:PRO:HA	1:24:A:PRO:HD2	7	0.25
(2,303)	1:3:A:GLU:HA	1:6:A:ARG:HB2	1	0.25
(2,248)	1:5:A:VAL:HB	1:6:A:ARG:H	7	0.25
(2,232)	1:7:A:LEU:H	1:8:A:TYR:HB3	6	0.25
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.25
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.25
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.25
(2,92)	1:24:A:PRO:HA	1:24:A:PRO:HD2	7	0.25
(2,28)	1:17:A:PRO:HA	1:17:A:PRO:HD2	10	0.25
(1,317)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	2	0.25
(1,317)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	7	0.25
(1,304)	1:3:A:GLU:HA	1:6:A:ARG:HB3	3	0.25
(1,275)	1:9:A:ILE:H	1:10:A:GLN:H	2	0.25
(1,275)	1:9:A:ILE:H	1:10:A:GLN:H	8	0.25
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB2	10	0.25
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD2	6	0.25
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD3	6	0.25
(1,197)	1:12:A:LEU:HA	1:12:A:LEU:HB2	5	0.25
(1,197)	1:12:A:LEU:HA	1:12:A:LEU:HB2	6	0.25
(1,197)	1:12:A:LEU:HA	1:12:A:LEU:HB2	7	0.25
(1,197)	1:12:A:LEU:HA	1:12:A:LEU:HB2	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:24:A:PRO:HA	1:25:A:SER:H	7	0.25
(1,137)	1:24:A:PRO:HA	1:25:A:SER:H	9	0.25
(1,125)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	3	0.25
(1,45)	1:21:A:ARG:HA	1:21:A:ARG:HB2	7	0.25
(1,20)	1:2:A:GLU:HA	1:3:A:GLU:H	2	0.25
(4,10)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.24
(3,237)	1:5:A:VAL:HB	1:6:A:ARG:H	8	0.24
(2,248)	1:5:A:VAL:HB	1:6:A:ARG:H	8	0.24
(2,240)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.24
(1,337)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	8	0.24
(1,337)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	8	0.24
(1,337)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	8	0.24
(1,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	8	0.24
(1,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	8	0.24
(1,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	8	0.24
(1,327)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	8	0.24
(1,327)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	8	0.24
(1,327)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	8	0.24
(1,317)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	1	0.24
(1,317)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	3	0.24
(1,281)	1:11:A:TRP:HE3	1:12:A:LEU:H	6	0.24
(1,275)	1:9:A:ILE:H	1:10:A:GLN:H	6	0.24
(1,275)	1:9:A:ILE:H	1:10:A:GLN:H	7	0.24
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB2	4	0.24
(1,227)	1:13:A:LYS:HA	1:14:A:GLN:H	9	0.24
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD2	2	0.24
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD3	2	0.24
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD2	10	0.24
(1,210)	1:13:A:LYS:HA	1:13:A:LYS:HD3	10	0.24
(1,197)	1:12:A:LEU:HA	1:12:A:LEU:HB2	1	0.24
(1,197)	1:12:A:LEU:HA	1:12:A:LEU:HB2	3	0.24
(1,197)	1:12:A:LEU:HA	1:12:A:LEU:HB2	4	0.24
(1,197)	1:12:A:LEU:HA	1:12:A:LEU:HB2	9	0.24
(1,197)	1:12:A:LEU:HA	1:12:A:LEU:HB2	10	0.24
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	1	0.24
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	1	0.24
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	1	0.24
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG11	9	0.24
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG12	9	0.24
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG13	9	0.24
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG21	9	0.24
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG22	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG23	9	0.24
(1,140)	1:11:A:TRP:H	1:12:A:LEU:H	5	0.24
(1,140)	1:11:A:TRP:H	1:12:A:LEU:H	6	0.24
(1,140)	1:11:A:TRP:H	1:12:A:LEU:H	8	0.24
(1,137)	1:24:A:PRO:HA	1:25:A:SER:H	1	0.24
(1,135)	1:14:A:GLN:H	1:14:A:GLN:HG2	7	0.24
(1,123)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	2	0.24
(4,10)	1:12:A:LEU:H	1:12:A:LEU:HG	7	0.23
(4,10)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.23
(4,10)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.23
(4,8)	1:7:A:LEU:H	1:8:A:TYR:HB3	7	0.23
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.23
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.23
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.23
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	4	0.23
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	4	0.23
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	4	0.23
(3,223)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.23
(2,240)	1:12:A:LEU:H	1:12:A:LEU:HG	7	0.23
(2,240)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.23
(2,240)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.23
(2,232)	1:7:A:LEU:H	1:8:A:TYR:HB3	7	0.23
(2,230)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.23
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.23
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.23
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.23
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD11	4	0.23
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD12	4	0.23
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD13	4	0.23
(1,317)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	10	0.23
(1,159)	1:7:A:LEU:HD11	1:7:A:LEU:HG	5	0.23
(1,159)	1:7:A:LEU:HD12	1:7:A:LEU:HG	5	0.23
(1,159)	1:7:A:LEU:HD13	1:7:A:LEU:HG	5	0.23
(1,152)	1:7:A:LEU:HA	1:7:A:LEU:HB2	8	0.23
(1,140)	1:11:A:TRP:H	1:12:A:LEU:H	2	0.23
(1,139)	1:5:A:VAL:H	1:6:A:ARG:H	9	0.23
(1,137)	1:24:A:PRO:HA	1:25:A:SER:H	6	0.23
(1,125)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	5	0.23
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG2	5	0.23
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG3	5	0.23
(4,10)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.22
(4,10)	1:12:A:LEU:H	1:12:A:LEU:HG	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,8)	1:7:A:LEU:H	1:8:A:TYR:HB3	8	0.22
(3,289)	1:3:A:GLU:HA	1:6:A:ARG:HB2	3	0.22
(3,276)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	4	0.22
(3,276)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	4	0.22
(2,303)	1:3:A:GLU:HA	1:6:A:ARG:HB2	3	0.22
(2,289)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	4	0.22
(2,289)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	4	0.22
(2,240)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.22
(2,240)	1:12:A:LEU:H	1:12:A:LEU:HG	3	0.22
(2,232)	1:7:A:LEU:H	1:8:A:TYR:HB3	8	0.22
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	6	0.22
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	6	0.22
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	6	0.22
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	6	0.22
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	6	0.22
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	6	0.22
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	6	0.22
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	6	0.22
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	6	0.22
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	6	0.22
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	6	0.22
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	6	0.22
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	6	0.22
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	6	0.22
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	6	0.22
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	6	0.22
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	6	0.22
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	6	0.22
(1,317)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	9	0.22
(1,259)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	3	0.22
(1,259)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	3	0.22
(1,242)	1:6:A:ARG:HB3	1:7:A:LEU:H	2	0.22
(1,194)	1:20:A:GLY:H	1:20:A:GLY:HA3	1	0.22
(1,194)	1:20:A:GLY:H	1:20:A:GLY:HA3	4	0.22
(1,194)	1:20:A:GLY:H	1:20:A:GLY:HA3	6	0.22
(1,194)	1:20:A:GLY:H	1:20:A:GLY:HA3	7	0.22
(1,171)	1:9:A:ILE:HA	1:9:A:ILE:HG12	3	0.22
(1,171)	1:9:A:ILE:HA	1:9:A:ILE:HG12	10	0.22
(1,159)	1:7:A:LEU:HD11	1:7:A:LEU:HG	4	0.22
(1,159)	1:7:A:LEU:HD12	1:7:A:LEU:HG	4	0.22
(1,159)	1:7:A:LEU:HD13	1:7:A:LEU:HG	4	0.22
(1,159)	1:7:A:LEU:HD11	1:7:A:LEU:HG	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:7:A:LEU:HD12	1:7:A:LEU:HG	8	0.22
(1,159)	1:7:A:LEU:HD13	1:7:A:LEU:HG	8	0.22
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG11	1	0.22
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG12	1	0.22
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG13	1	0.22
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG21	1	0.22
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG22	1	0.22
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG23	1	0.22
(1,137)	1:24:A:PRO:HA	1:25:A:SER:H	10	0.22
(1,125)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	1	0.22
(1,113)	1:6:A:ARG:HA	1:6:A:ARG:HB2	2	0.22
(1,112)	1:6:A:ARG:HA	1:6:A:ARG:HB3	10	0.22
(1,106)	1:6:A:ARG:HA	1:6:A:ARG:HG2	3	0.22
(1,57)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	3	0.22
(1,57)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	4	0.22
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG2	1	0.22
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG3	1	0.22
(4,10)	1:12:A:LEU:H	1:12:A:LEU:HG	5	0.21
(4,4)	1:24:A:PRO:HA	1:24:A:PRO:HD3	7	0.21
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD21	5	0.21
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD22	5	0.21
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD23	5	0.21
(3,237)	1:5:A:VAL:HB	1:6:A:ARG:H	10	0.21
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.21
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.21
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.21
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD21	5	0.21
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD22	5	0.21
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD23	5	0.21
(2,248)	1:5:A:VAL:HB	1:6:A:ARG:H	10	0.21
(2,240)	1:12:A:LEU:H	1:12:A:LEU:HG	5	0.21
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.21
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.21
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.21
(2,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	7	0.21
(1,330)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	1	0.21
(1,330)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	1	0.21
(1,330)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	1	0.21
(1,296)	1:8:A:TYR:HA	1:24:A:PRO:HD3	1	0.21
(1,281)	1:11:A:TRP:HE3	1:12:A:LEU:H	1	0.21
(1,279)	1:19:A:SER:H	1:20:A:GLY:H	8	0.21
(1,255)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	5	0.21
(1,194)	1:20:A:GLY:H	1:20:A:GLY:HA3	2	0.21
(1,194)	1:20:A:GLY:H	1:20:A:GLY:HA3	3	0.21
(1,171)	1:9:A:ILE:HA	1:9:A:ILE:HG12	4	0.21
(1,159)	1:7:A:LEU:HD11	1:7:A:LEU:HG	6	0.21
(1,159)	1:7:A:LEU:HD12	1:7:A:LEU:HG	6	0.21
(1,159)	1:7:A:LEU:HD13	1:7:A:LEU:HG	6	0.21
(1,159)	1:7:A:LEU:HD11	1:7:A:LEU:HG	7	0.21
(1,159)	1:7:A:LEU:HD12	1:7:A:LEU:HG	7	0.21
(1,159)	1:7:A:LEU:HD13	1:7:A:LEU:HG	7	0.21
(1,130)	1:14:A:GLN:HA	1:14:A:GLN:HG3	10	0.21
(1,125)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	8	0.21
(1,115)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	7	0.21
(1,110)	1:6:A:ARG:H	1:6:A:ARG:HG3	8	0.21
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB2	5	0.21
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB3	5	0.21
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG2	3	0.21
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG3	3	0.21
(1,7)	1:3:A:GLU:HA	1:4:A:ALA:H	6	0.21
(4,10)	1:12:A:LEU:H	1:12:A:LEU:HG	6	0.2
(3,315)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	6	0.2
(3,315)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	6	0.2
(3,315)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	6	0.2
(3,237)	1:5:A:VAL:HB	1:6:A:ARG:H	4	0.2
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD11	2	0.2
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD12	2	0.2
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD13	2	0.2
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD11	7	0.2
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD12	7	0.2
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD13	7	0.2
(2,330)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	6	0.2
(2,330)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	6	0.2
(2,330)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	6	0.2
(2,248)	1:5:A:VAL:HB	1:6:A:ARG:H	4	0.2
(2,240)	1:12:A:LEU:H	1:12:A:LEU:HG	6	0.2
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	2	0.2
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	2	0.2
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	2	0.2
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	7	0.2
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	7	0.2
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	7	0.2
(1,317)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	6	0.2
(1,298)	1:8:A:TYR:HA	1:8:A:TYR:HB2	4	0.2
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	9	0.2
(1,256)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	9	0.2
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	9	0.2
(1,256)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	9	0.2
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	9	0.2
(1,256)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	9	0.2
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	9	0.2
(1,256)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	9	0.2
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	9	0.2
(1,256)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	9	0.2
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	9	0.2
(1,256)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	9	0.2
(1,194)	1:20:A:GLY:H	1:20:A:GLY:HA3	9	0.2
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	1	0.2
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	1	0.2
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	5	0.2
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	5	0.2
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	5	0.2
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.2
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.2
(1,156)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.2
(1,139)	1:5:A:VAL:H	1:6:A:ARG:H	4	0.2
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB2	3	0.2
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB3	3	0.2
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB2	6	0.2
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB3	6	0.2
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB2	7	0.2
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB3	7	0.2
(1,57)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	1	0.2
(1,57)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	2	0.2
(1,57)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	9	0.2
(1,57)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	10	0.2
(1,56)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	6	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	1	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	1	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	2	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	2	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	4	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	4	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	5	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	6	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	6	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	9	0.2
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	9	0.2
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD2	10	0.2
(1,40)	1:21:A:ARG:HA	1:21:A:ARG:HD3	10	0.2
(4,8)	1:7:A:LEU:H	1:8:A:TYR:HB3	4	0.19
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	8	0.19
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	8	0.19
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	8	0.19
(4,4)	1:24:A:PRO:HA	1:24:A:PRO:HD3	9	0.19
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.19
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.19
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.19
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.19
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.19
(3,156)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.19
(3,130)	1:14:A:GLN:H	1:14:A:GLN:HG2	2	0.19
(3,130)	1:14:A:GLN:H	1:14:A:GLN:HG2	6	0.19
(2,232)	1:7:A:LEU:H	1:8:A:TYR:HB3	4	0.19
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.19
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.19
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.19
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.19
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.19
(2,163)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.19
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD11	8	0.19
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD12	8	0.19
(2,155)	1:7:A:LEU:HA	1:7:A:LEU:HD13	8	0.19
(2,135)	1:14:A:GLN:H	1:14:A:GLN:HG2	2	0.19
(2,135)	1:14:A:GLN:H	1:14:A:GLN:HG2	6	0.19
(2,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	9	0.19
(1,335)	1:7:A:LEU:HD11	1:8:A:TYR:HB2	2	0.19
(1,335)	1:7:A:LEU:HD12	1:8:A:TYR:HB2	2	0.19
(1,335)	1:7:A:LEU:HD13	1:8:A:TYR:HB2	2	0.19
(1,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	10	0.19
(1,274)	1:6:A:ARG:H	1:7:A:LEU:H	9	0.19
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB2	9	0.19
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB3	9	0.19
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	4	0.19
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	7	0.19
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	7	0.19
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	2	0.19
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	2	0.19
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	2	0.19
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	9	0.19
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	9	0.19
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	9	0.19
(1,159)	1:7:A:LEU:HD11	1:7:A:LEU:HG	1	0.19
(1,159)	1:7:A:LEU:HD12	1:7:A:LEU:HG	1	0.19
(1,159)	1:7:A:LEU:HD13	1:7:A:LEU:HG	1	0.19
(1,159)	1:7:A:LEU:HD11	1:7:A:LEU:HG	2	0.19
(1,159)	1:7:A:LEU:HD12	1:7:A:LEU:HG	2	0.19
(1,159)	1:7:A:LEU:HD13	1:7:A:LEU:HG	2	0.19
(1,159)	1:7:A:LEU:HD11	1:7:A:LEU:HG	3	0.19
(1,159)	1:7:A:LEU:HD12	1:7:A:LEU:HG	3	0.19
(1,159)	1:7:A:LEU:HD13	1:7:A:LEU:HG	3	0.19
(1,159)	1:7:A:LEU:HD11	1:7:A:LEU:HG	9	0.19
(1,159)	1:7:A:LEU:HD12	1:7:A:LEU:HG	9	0.19
(1,159)	1:7:A:LEU:HD13	1:7:A:LEU:HG	9	0.19
(1,159)	1:7:A:LEU:HD11	1:7:A:LEU:HG	10	0.19
(1,159)	1:7:A:LEU:HD12	1:7:A:LEU:HG	10	0.19
(1,159)	1:7:A:LEU:HD13	1:7:A:LEU:HG	10	0.19
(1,142)	1:12:A:LEU:H	1:13:A:LYS:H	3	0.19
(1,137)	1:24:A:PRO:HA	1:25:A:SER:H	4	0.19
(1,125)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	7	0.19
(1,125)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	9	0.19
(1,115)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	4	0.19
(1,109)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.19
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB2	4	0.19
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB3	4	0.19
(1,57)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	7	0.19
(1,57)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	8	0.19
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	3	0.19
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	3	0.19
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	8	0.19
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	8	0.19
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	10	0.19
(1,48)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	10	0.19
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG2	7	0.19
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG3	7	0.19
(4,13)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,13)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	3	0.18
(4,13)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	4	0.18
(4,13)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	5	0.18
(4,13)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	6	0.18
(4,13)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	7	0.18
(4,13)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	8	0.18
(4,11)	1:7:A:LEU:HB2	1:8:A:TYR:H	2	0.18
(3,307)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	1	0.18
(3,307)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	4	0.18
(3,169)	1:9:A:ILE:H	1:9:A:ILE:HG12	7	0.18
(3,130)	1:14:A:GLN:H	1:14:A:GLN:HG2	4	0.18
(3,89)	1:24:A:PRO:HA	1:24:A:PRO:HD2	8	0.18
(2,322)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	1	0.18
(2,322)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	4	0.18
(2,265)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	2	0.18
(2,265)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	3	0.18
(2,265)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	4	0.18
(2,265)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	5	0.18
(2,265)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	6	0.18
(2,265)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	7	0.18
(2,265)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	8	0.18
(2,245)	1:7:A:LEU:HB2	1:8:A:TYR:H	2	0.18
(2,176)	1:9:A:ILE:H	1:9:A:ILE:HG12	7	0.18
(2,135)	1:14:A:GLN:H	1:14:A:GLN:HG2	4	0.18
(2,92)	1:24:A:PRO:HA	1:24:A:PRO:HD2	8	0.18
(1,283)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	3	0.18
(1,283)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	9	0.18
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB2	5	0.18
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB3	5	0.18
(1,130)	1:14:A:GLN:HA	1:14:A:GLN:HG3	9	0.18
(1,125)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	10	0.18
(1,124)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	7	0.18
(1,109)	1:6:A:ARG:H	1:6:A:ARG:HB3	1	0.18
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB2	9	0.18
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB3	9	0.18
(1,96)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	1	0.18
(1,96)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	2	0.18
(1,96)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	4	0.18
(1,96)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	5	0.18
(1,96)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	8	0.18
(1,96)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	9	0.18
(1,96)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	1	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	1	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	2	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	2	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	3	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	3	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	4	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	4	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	5	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	5	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	7	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	7	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	8	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	8	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	9	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	9	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	10	0.18
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	10	0.18
(4,13)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	1	0.17
(4,13)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	9	0.17
(4,13)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	10	0.17
(4,8)	1:7:A:LEU:H	1:8:A:TYR:HB3	2	0.17
(4,4)	1:24:A:PRO:HA	1:24:A:PRO:HD3	10	0.17
(3,315)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	9	0.17
(3,315)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	9	0.17
(3,315)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	9	0.17
(3,307)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	2	0.17
(3,307)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	9	0.17
(3,229)	1:3:A:GLU:H	1:3:A:GLU:HB2	5	0.17
(3,90)	1:11:A:TRP:HA	1:11:A:TRP:HB3	9	0.17
(2,330)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	9	0.17
(2,330)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	9	0.17
(2,330)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	9	0.17
(2,322)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	2	0.17
(2,322)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	9	0.17
(2,265)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	1	0.17
(2,265)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	9	0.17
(2,265)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	10	0.17
(2,238)	1:3:A:GLU:H	1:3:A:GLU:HB2	5	0.17
(2,232)	1:7:A:LEU:H	1:8:A:TYR:HB3	2	0.17
(2,95)	1:11:A:TRP:HA	1:11:A:TRP:HB3	9	0.17
(2,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB2	1	0.17
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB3	1	0.17
(1,283)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	1	0.17
(1,283)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	8	0.17
(1,280)	1:4:A:ALA:H	1:5:A:VAL:H	3	0.17
(1,255)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	1	0.17
(1,255)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	1	0.17
(1,244)	1:12:A:LEU:HB2	1:13:A:LYS:H	1	0.17
(1,244)	1:12:A:LEU:HB2	1:13:A:LYS:H	8	0.17
(1,244)	1:12:A:LEU:HB2	1:13:A:LYS:H	10	0.17
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB2	8	0.17
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB3	8	0.17
(1,219)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	5	0.17
(1,219)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	5	0.17
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	3	0.17
(1,215)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	3	0.17
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	3	0.17
(1,215)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	3	0.17
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	10	0.17
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	10	0.17
(1,171)	1:9:A:ILE:HA	1:9:A:ILE:HG12	8	0.17
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG2	6	0.17
(1,147)	1:3:A:GLU:HA	1:3:A:GLU:HG3	6	0.17
(1,114)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	3	0.17
(1,112)	1:6:A:ARG:HA	1:6:A:ARG:HB3	7	0.17
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB2	2	0.17
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB3	2	0.17
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB2	8	0.17
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB3	8	0.17
(1,96)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	3	0.17
(1,96)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	6	0.17
(1,96)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	7	0.17
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG2	2	0.17
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG3	2	0.17
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG2	9	0.17
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG3	9	0.17
(4,15)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	5	0.16
(4,15)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	6	0.16
(4,11)	1:7:A:LEU:HB2	1:8:A:TYR:H	4	0.16
(4,4)	1:24:A:PRO:HA	1:24:A:PRO:HD3	6	0.16
(3,316)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	6	0.16
(3,316)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,316)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	6	0.16
(3,307)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	3	0.16
(3,289)	1:3:A:GLU:HA	1:6:A:ARG:HB2	9	0.16
(3,265)	1:10:A:GLN:H	1:11:A:TRP:H	1	0.16
(3,232)	1:6:A:ARG:HB3	1:7:A:LEU:H	10	0.16
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD11	5	0.16
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD12	5	0.16
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD13	5	0.16
(3,103)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.16
(3,90)	1:11:A:TRP:HA	1:11:A:TRP:HB3	2	0.16
(3,90)	1:11:A:TRP:HA	1:11:A:TRP:HB3	3	0.16
(3,90)	1:11:A:TRP:HA	1:11:A:TRP:HB3	4	0.16
(3,90)	1:11:A:TRP:HA	1:11:A:TRP:HB3	5	0.16
(3,90)	1:11:A:TRP:HA	1:11:A:TRP:HB3	6	0.16
(3,90)	1:11:A:TRP:HA	1:11:A:TRP:HB3	7	0.16
(3,90)	1:11:A:TRP:HA	1:11:A:TRP:HB3	8	0.16
(3,90)	1:11:A:TRP:HA	1:11:A:TRP:HB3	10	0.16
(2,331)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	6	0.16
(2,331)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	6	0.16
(2,331)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	6	0.16
(2,322)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	3	0.16
(2,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	5	0.16
(2,311)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	6	0.16
(2,303)	1:3:A:GLU:HA	1:6:A:ARG:HB2	9	0.16
(2,278)	1:10:A:GLN:H	1:11:A:TRP:H	1	0.16
(2,245)	1:7:A:LEU:HB2	1:8:A:TYR:H	4	0.16
(2,242)	1:6:A:ARG:HB3	1:7:A:LEU:H	10	0.16
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	5	0.16
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	5	0.16
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	5	0.16
(2,108)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.16
(2,95)	1:11:A:TRP:HA	1:11:A:TRP:HB3	2	0.16
(2,95)	1:11:A:TRP:HA	1:11:A:TRP:HB3	3	0.16
(2,95)	1:11:A:TRP:HA	1:11:A:TRP:HB3	4	0.16
(2,95)	1:11:A:TRP:HA	1:11:A:TRP:HB3	5	0.16
(2,95)	1:11:A:TRP:HA	1:11:A:TRP:HB3	6	0.16
(2,95)	1:11:A:TRP:HA	1:11:A:TRP:HB3	7	0.16
(2,95)	1:11:A:TRP:HA	1:11:A:TRP:HB3	8	0.16
(2,95)	1:11:A:TRP:HA	1:11:A:TRP:HB3	10	0.16
(2,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	6	0.16
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD11	7	0.16
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD12	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:4:A:ALA:HA	1:7:A:LEU:HD13	7	0.16
(1,300)	1:23:A:PRO:HA	1:24:A:PRO:HD3	8	0.16
(1,251)	1:13:A:LYS:HB2	1:14:A:GLN:H	3	0.16
(1,251)	1:13:A:LYS:HB3	1:14:A:GLN:H	3	0.16
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	3	0.16
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	3	0.16
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	6	0.16
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	6	0.16
(1,154)	1:7:A:LEU:HA	1:7:A:LEU:HB3	3	0.16
(1,154)	1:7:A:LEU:HA	1:7:A:LEU:HB3	10	0.16
(1,137)	1:24:A:PRO:HA	1:25:A:SER:H	2	0.16
(1,112)	1:6:A:ARG:HA	1:6:A:ARG:HB3	8	0.16
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB2	10	0.16
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB3	10	0.16
(1,51)	1:22:A:PRO:HA	1:22:A:PRO:HD3	6	0.16
(1,14)	1:8:A:TYR:H	1:8:A:TYR:HA	2	0.16
(4,3)	1:22:A:PRO:HA	1:22:A:PRO:HD3	9	0.15
(3,312)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	8	0.15
(3,312)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	8	0.15
(3,312)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	8	0.15
(3,307)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	8	0.15
(3,287)	1:23:A:PRO:HA	1:24:A:PRO:HD3	7	0.15
(3,265)	1:10:A:GLN:H	1:11:A:TRP:H	6	0.15
(3,265)	1:10:A:GLN:H	1:11:A:TRP:H	8	0.15
(3,235)	1:21:A:ARG:H	1:21:A:ARG:HB3	4	0.15
(3,229)	1:3:A:GLU:H	1:3:A:GLU:HB2	9	0.15
(3,162)	1:7:A:LEU:H	1:7:A:LEU:HD21	2	0.15
(3,162)	1:7:A:LEU:H	1:7:A:LEU:HD22	2	0.15
(3,162)	1:7:A:LEU:H	1:7:A:LEU:HD23	2	0.15
(3,161)	1:7:A:LEU:H	1:7:A:LEU:HD11	7	0.15
(3,161)	1:7:A:LEU:H	1:7:A:LEU:HD12	7	0.15
(3,161)	1:7:A:LEU:H	1:7:A:LEU:HD13	7	0.15
(3,90)	1:11:A:TRP:HA	1:11:A:TRP:HB3	1	0.15
(2,327)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	8	0.15
(2,327)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	8	0.15
(2,327)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	8	0.15
(2,322)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	8	0.15
(2,300)	1:23:A:PRO:HA	1:24:A:PRO:HD3	7	0.15
(2,278)	1:10:A:GLN:H	1:11:A:TRP:H	6	0.15
(2,278)	1:10:A:GLN:H	1:11:A:TRP:H	8	0.15
(2,246)	1:21:A:ARG:H	1:21:A:ARG:HB3	4	0.15
(2,238)	1:3:A:GLU:H	1:3:A:GLU:HB2	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,169)	1:7:A:LEU:H	1:7:A:LEU:HD21	2	0.15
(2,169)	1:7:A:LEU:H	1:7:A:LEU:HD22	2	0.15
(2,169)	1:7:A:LEU:H	1:7:A:LEU:HD23	2	0.15
(2,168)	1:7:A:LEU:H	1:7:A:LEU:HD11	7	0.15
(2,168)	1:7:A:LEU:H	1:7:A:LEU:HD12	7	0.15
(2,168)	1:7:A:LEU:H	1:7:A:LEU:HD13	7	0.15
(2,95)	1:11:A:TRP:HA	1:11:A:TRP:HB3	1	0.15
(2,51)	1:22:A:PRO:HA	1:22:A:PRO:HD3	9	0.15
(1,298)	1:8:A:TYR:HA	1:8:A:TYR:HB2	3	0.15
(1,296)	1:8:A:TYR:HA	1:24:A:PRO:HD3	3	0.15
(1,226)	1:16:A:GLY:H	1:16:A:GLY:HA2	3	0.15
(1,192)	1:11:A:TRP:H	1:11:A:TRP:HB3	2	0.15
(1,192)	1:11:A:TRP:H	1:11:A:TRP:HB3	7	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG21	1	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG22	1	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG23	1	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG21	2	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG22	2	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG23	2	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG21	3	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG22	3	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG23	3	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG21	4	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG22	4	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG23	4	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG21	5	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG22	5	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG23	5	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG21	6	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG22	6	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG23	6	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG21	7	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG22	7	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG23	7	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG21	8	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG22	8	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG23	8	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG21	9	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG22	9	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG23	9	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG21	10	0.15
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG22	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:9:A:ILE:HB	1:9:A:ILE:HG23	10	0.15
(1,171)	1:9:A:ILE:HA	1:9:A:ILE:HG12	6	0.15
(1,152)	1:7:A:LEU:HA	1:7:A:LEU:HB2	7	0.15
(1,137)	1:24:A:PRO:HA	1:25:A:SER:H	5	0.15
(1,130)	1:14:A:GLN:HA	1:14:A:GLN:HG3	6	0.15
(1,129)	1:14:A:GLN:HA	1:14:A:GLN:HG2	7	0.15
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB2	1	0.15
(1,100)	1:10:A:GLN:HA	1:10:A:GLN:HB3	1	0.15
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG2	4	0.15
(1,30)	1:17:A:PRO:HA	1:17:A:PRO:HG3	4	0.15
(1,14)	1:8:A:TYR:H	1:8:A:TYR:HA	7	0.15
(1,13)	1:12:A:LEU:H	1:12:A:LEU:HA	5	0.15
(1,13)	1:12:A:LEU:H	1:12:A:LEU:HA	7	0.15
(1,13)	1:12:A:LEU:H	1:12:A:LEU:HA	8	0.15
(4,3)	1:22:A:PRO:HA	1:22:A:PRO:HD3	4	0.14
(4,3)	1:22:A:PRO:HA	1:22:A:PRO:HD3	8	0.14
(3,265)	1:10:A:GLN:H	1:11:A:TRP:H	4	0.14
(3,265)	1:10:A:GLN:H	1:11:A:TRP:H	7	0.14
(3,265)	1:10:A:GLN:H	1:11:A:TRP:H	10	0.14
(3,232)	1:6:A:ARG:HB3	1:7:A:LEU:H	7	0.14
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.14
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.14
(3,167)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.14
(3,53)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	3	0.14
(3,53)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	4	0.14
(2,278)	1:10:A:GLN:H	1:11:A:TRP:H	4	0.14
(2,278)	1:10:A:GLN:H	1:11:A:TRP:H	7	0.14
(2,278)	1:10:A:GLN:H	1:11:A:TRP:H	10	0.14
(2,242)	1:6:A:ARG:HB3	1:7:A:LEU:H	7	0.14
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.14
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.14
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.14
(2,56)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	3	0.14
(2,56)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	4	0.14
(2,51)	1:22:A:PRO:HA	1:22:A:PRO:HD3	4	0.14
(2,51)	1:22:A:PRO:HA	1:22:A:PRO:HD3	8	0.14
(1,335)	1:7:A:LEU:HD11	1:8:A:TYR:HB2	4	0.14
(1,335)	1:7:A:LEU:HD12	1:8:A:TYR:HB2	4	0.14
(1,335)	1:7:A:LEU:HD13	1:8:A:TYR:HB2	4	0.14
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	4	0.14
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	4	0.14
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	4	0.14
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	4	0.14
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	4	0.14
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	4	0.14
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	4	0.14
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	4	0.14
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	4	0.14
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	4	0.14
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	4	0.14
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	4	0.14
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	4	0.14
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	4	0.14
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	4	0.14
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	4	0.14
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	4	0.14
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB2	7	0.14
(1,307)	1:10:A:GLN:HA	1:13:A:LYS:HB3	7	0.14
(1,304)	1:3:A:GLU:HA	1:6:A:ARG:HB3	9	0.14
(1,298)	1:8:A:TYR:HA	1:8:A:TYR:HB2	1	0.14
(1,298)	1:8:A:TYR:HA	1:8:A:TYR:HB2	7	0.14
(1,298)	1:8:A:TYR:HA	1:8:A:TYR:HB2	10	0.14
(1,297)	1:8:A:TYR:HA	1:11:A:TRP:HB3	7	0.14
(1,283)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	2	0.14
(1,260)	1:4:A:ALA:HB1	1:5:A:VAL:H	10	0.14
(1,260)	1:4:A:ALA:HB2	1:5:A:VAL:H	10	0.14
(1,260)	1:4:A:ALA:HB3	1:5:A:VAL:H	10	0.14
(1,237)	1:3:A:GLU:H	1:3:A:GLU:HB3	5	0.14
(1,226)	1:16:A:GLY:H	1:16:A:GLY:HA2	7	0.14
(1,192)	1:11:A:TRP:H	1:11:A:TRP:HB3	4	0.14
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	2	0.14
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	2	0.14
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD11	8	0.14
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD12	8	0.14
(1,168)	1:7:A:LEU:H	1:7:A:LEU:HD13	8	0.14
(1,154)	1:7:A:LEU:HA	1:7:A:LEU:HB3	1	0.14
(1,124)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	2	0.14
(1,124)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	10	0.14
(1,46)	1:21:A:ARG:HA	1:21:A:ARG:HG2	1	0.14
(1,46)	1:21:A:ARG:HA	1:21:A:ARG:HG3	1	0.14
(1,14)	1:8:A:TYR:H	1:8:A:TYR:HA	6	0.14
(1,13)	1:12:A:LEU:H	1:12:A:LEU:HA	2	0.14
(1,13)	1:12:A:LEU:H	1:12:A:LEU:HA	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	1	0.14
(1,3)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	2	0.14
(1,3)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	3	0.14
(1,3)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	4	0.14
(1,3)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	5	0.14
(1,3)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	6	0.14
(1,3)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	7	0.14
(1,3)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	8	0.14
(1,3)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	9	0.14
(1,3)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	10	0.14
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD21	9	0.13
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD22	9	0.13
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD23	9	0.13
(3,307)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	5	0.13
(3,299)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	9	0.13
(3,294)	1:9:A:ILE:HA	1:12:A:LEU:HB3	2	0.13
(3,288)	1:8:A:TYR:HB2	1:24:A:PRO:HD2	2	0.13
(3,274)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.13
(3,265)	1:10:A:GLN:H	1:11:A:TRP:H	3	0.13
(3,265)	1:10:A:GLN:H	1:11:A:TRP:H	5	0.13
(3,265)	1:10:A:GLN:H	1:11:A:TRP:H	9	0.13
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.13
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.13
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.13
(3,53)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	1	0.13
(3,53)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	9	0.13
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD21	9	0.13
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD22	9	0.13
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD23	9	0.13
(2,322)	1:16:A:GLY:HA2	1:21:A:ARG:HB3	5	0.13
(2,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	9	0.13
(2,308)	1:9:A:ILE:HA	1:12:A:LEU:HB3	2	0.13
(2,301)	1:8:A:TYR:HB2	1:24:A:PRO:HD2	2	0.13
(2,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.13
(2,278)	1:10:A:GLN:H	1:11:A:TRP:H	3	0.13
(2,278)	1:10:A:GLN:H	1:11:A:TRP:H	5	0.13
(2,278)	1:10:A:GLN:H	1:11:A:TRP:H	9	0.13
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.13
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.13
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.13
(2,56)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	1	0.13
(2,56)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	1	0.13
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	1	0.13
(1,323)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	1	0.13
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	1	0.13
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	1	0.13
(1,323)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	1	0.13
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	1	0.13
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	1	0.13
(1,323)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	1	0.13
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	1	0.13
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	1	0.13
(1,323)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	1	0.13
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	1	0.13
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	1	0.13
(1,323)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	1	0.13
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	1	0.13
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	1	0.13
(1,323)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	1	0.13
(1,297)	1:8:A:TYR:HA	1:11:A:TRP:HB3	9	0.13
(1,281)	1:11:A:TRP:HE3	1:12:A:LEU:H	9	0.13
(1,255)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	2	0.13
(1,255)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	2	0.13
(1,248)	1:5:A:VAL:HB	1:6:A:ARG:H	1	0.13
(1,226)	1:16:A:GLY:H	1:16:A:GLY:HA2	4	0.13
(1,201)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	2	0.13
(1,201)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	3	0.13
(1,201)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	4	0.13
(1,201)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	5	0.13
(1,201)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	6	0.13
(1,201)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	7	0.13
(1,201)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	8	0.13
(1,201)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.13
(1,192)	1:11:A:TRP:H	1:11:A:TRP:HB3	1	0.13
(1,192)	1:11:A:TRP:H	1:11:A:TRP:HB3	6	0.13
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	5	0.13
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	5	0.13
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG11	6	0.13
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG12	6	0.13
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG13	6	0.13
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG21	6	0.13
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG22	6	0.13
(1,146)	1:5:A:VAL:HA	1:5:A:VAL:HG23	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB2	1	0.13
(1,136)	1:14:A:GLN:H	1:14:A:GLN:HB3	1	0.13
(1,119)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	6	0.13
(1,53)	1:22:A:PRO:HA	1:22:A:PRO:HB2	5	0.13
(1,26)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	9	0.13
(1,13)	1:12:A:LEU:H	1:12:A:LEU:HA	1	0.13
(1,13)	1:12:A:LEU:H	1:12:A:LEU:HA	6	0.13
(4,4)	1:24:A:PRO:HA	1:24:A:PRO:HD3	1	0.12
(4,3)	1:22:A:PRO:HA	1:22:A:PRO:HD3	1	0.12
(4,3)	1:22:A:PRO:HA	1:22:A:PRO:HD3	3	0.12
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD21	10	0.12
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD22	10	0.12
(3,325)	1:4:A:ALA:HA	1:7:A:LEU:HD23	10	0.12
(3,294)	1:9:A:ILE:HA	1:12:A:LEU:HB3	3	0.12
(3,286)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	2	0.12
(3,235)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.12
(3,213)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	9	0.12
(3,213)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.12
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.12
(3,103)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.12
(3,89)	1:24:A:PRO:HA	1:24:A:PRO:HD2	10	0.12
(3,53)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	2	0.12
(3,53)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	8	0.12
(3,53)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	10	0.12
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD21	10	0.12
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD22	10	0.12
(2,340)	1:4:A:ALA:HA	1:7:A:LEU:HD23	10	0.12
(2,308)	1:9:A:ILE:HA	1:12:A:LEU:HB3	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,299)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	2	0.12
(2,246)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.12
(2,220)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	9	0.12
(2,220)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.12
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.12
(2,108)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.12
(2,93)	1:24:A:PRO:HA	1:24:A:PRO:HD3	1	0.12
(2,92)	1:24:A:PRO:HA	1:24:A:PRO:HD2	10	0.12
(2,56)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	2	0.12
(2,56)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	8	0.12
(2,56)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	10	0.12
(2,51)	1:22:A:PRO:HA	1:22:A:PRO:HD3	1	0.12
(2,51)	1:22:A:PRO:HA	1:22:A:PRO:HD3	3	0.12
(1,331)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	3	0.12
(1,331)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	3	0.12
(1,331)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	3	0.12
(1,306)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.12
(1,306)	1:7:A:LEU:HA	1:10:A:GLN:HB3	2	0.12
(1,300)	1:23:A:PRO:HA	1:24:A:PRO:HD3	4	0.12
(1,297)	1:8:A:TYR:HA	1:11:A:TRP:HB3	6	0.12
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB2	4	0.12
(1,243)	1:13:A:LYS:H	1:13:A:LYS:HB3	4	0.12
(1,226)	1:16:A:GLY:H	1:16:A:GLY:HA2	1	0.12
(1,201)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	1	0.12
(1,201)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	9	0.12
(1,192)	1:11:A:TRP:H	1:11:A:TRP:HB3	5	0.12
(1,192)	1:11:A:TRP:H	1:11:A:TRP:HB3	8	0.12
(1,192)	1:11:A:TRP:H	1:11:A:TRP:HB3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	7	0.12
(1,187)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	7	0.12
(1,187)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	7	0.12
(1,154)	1:7:A:LEU:HA	1:7:A:LEU:HB3	7	0.12
(1,152)	1:7:A:LEU:HA	1:7:A:LEU:HB2	6	0.12
(1,152)	1:7:A:LEU:HA	1:7:A:LEU:HB2	10	0.12
(1,119)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	10	0.12
(1,85)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	4	0.12
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	6	0.12
(1,62)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	6	0.12
(1,26)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	1	0.12
(1,26)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	2	0.12
(1,26)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	3	0.12
(1,26)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	4	0.12
(1,26)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	5	0.12
(1,26)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	6	0.12
(1,26)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	7	0.12
(1,26)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	8	0.12
(1,26)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.12
(3,322)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	9	0.11
(3,322)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	9	0.11
(3,322)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	9	0.11
(3,299)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	5	0.11
(3,294)	1:9:A:ILE:HA	1:12:A:LEU:HB3	6	0.11
(3,294)	1:9:A:ILE:HA	1:12:A:LEU:HB3	8	0.11
(3,287)	1:23:A:PRO:HA	1:24:A:PRO:HD3	2	0.11
(3,276)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	3	0.11
(3,276)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	3	0.11
(3,240)	1:13:A:LYS:HB2	1:14:A:GLN:H	9	0.11
(3,240)	1:13:A:LYS:HB3	1:14:A:GLN:H	9	0.11
(3,235)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.11
(3,232)	1:6:A:ARG:HB3	1:7:A:LEU:H	8	0.11
(3,228)	1:3:A:GLU:H	1:3:A:GLU:HB3	7	0.11
(3,213)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	8	0.11
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.11
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.11
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.11
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.11
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.11
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.11
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.11
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.11
(3,106)	1:6:A:ARG:H	1:6:A:ARG:HG2	2	0.11
(3,103)	1:6:A:ARG:H	1:6:A:ARG:HB2	8	0.11
(3,89)	1:24:A:PRO:HA	1:24:A:PRO:HD2	4	0.11
(3,89)	1:24:A:PRO:HA	1:24:A:PRO:HD2	5	0.11
(3,89)	1:24:A:PRO:HA	1:24:A:PRO:HD2	9	0.11
(3,53)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	5	0.11
(3,53)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	7	0.11
(3,15)	1:8:A:TYR:H	1:8:A:TYR:HB2	4	0.11
(2,337)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	9	0.11
(2,337)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	9	0.11
(2,337)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	9	0.11
(2,314)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	5	0.11
(2,308)	1:9:A:ILE:HA	1:12:A:LEU:HB3	6	0.11
(2,308)	1:9:A:ILE:HA	1:12:A:LEU:HB3	8	0.11
(2,300)	1:23:A:PRO:HA	1:24:A:PRO:HD3	2	0.11
(2,289)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	3	0.11
(2,289)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	3	0.11
(2,251)	1:13:A:LYS:HB2	1:14:A:GLN:H	9	0.11
(2,251)	1:13:A:LYS:HB3	1:14:A:GLN:H	9	0.11
(2,246)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.11
(2,242)	1:6:A:ARG:HB3	1:7:A:LEU:H	8	0.11
(2,237)	1:3:A:GLU:H	1:3:A:GLU:HB3	7	0.11
(2,220)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	8	0.11
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.11
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.11
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.11
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.11
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.11
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.11
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.11
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.11
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.11
(2,111)	1:6:A:ARG:H	1:6:A:ARG:HG2	2	0.11
(2,108)	1:6:A:ARG:H	1:6:A:ARG:HB2	8	0.11
(2,92)	1:24:A:PRO:HA	1:24:A:PRO:HD2	4	0.11
(2,92)	1:24:A:PRO:HA	1:24:A:PRO:HD2	5	0.11
(2,92)	1:24:A:PRO:HA	1:24:A:PRO:HD2	9	0.11
(2,56)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	5	0.11
(2,56)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	7	0.11
(2,15)	1:8:A:TYR:H	1:8:A:TYR:HB2	4	0.11
(1,298)	1:8:A:TYR:HA	1:8:A:TYR:HB2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:8:A:TYR:HA	1:8:A:TYR:HB2	9	0.11
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	4	0.11
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	4	0.11
(1,258)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	4	0.11
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	4	0.11
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	4	0.11
(1,258)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	4	0.11
(1,240)	1:12:A:LEU:H	1:12:A:LEU:HG	4	0.11
(1,226)	1:16:A:GLY:H	1:16:A:GLY:HA2	2	0.11
(1,189)	1:8:A:TYR:HB3	1:8:A:TYR:HD1	9	0.11
(1,189)	1:8:A:TYR:HB3	1:8:A:TYR:HD2	9	0.11
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	8	0.11
(1,188)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	8	0.11
(1,187)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	1	0.11
(1,187)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	1	0.11
(1,187)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	1	0.11
(1,187)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	2	0.11
(1,187)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	2	0.11
(1,187)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	2	0.11
(1,187)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	3	0.11
(1,187)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	3	0.11
(1,187)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	3	0.11
(1,187)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	4	0.11
(1,187)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	4	0.11
(1,187)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	4	0.11
(1,187)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	5	0.11
(1,187)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	5	0.11
(1,187)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	5	0.11
(1,187)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	6	0.11
(1,187)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	6	0.11
(1,187)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	6	0.11
(1,187)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	8	0.11
(1,187)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	8	0.11
(1,187)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	8	0.11
(1,187)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	9	0.11
(1,187)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	9	0.11
(1,187)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	9	0.11
(1,187)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	10	0.11
(1,187)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	10	0.11
(1,187)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	10	0.11
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	4	0.11
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	4	0.11
(1,152)	1:7:A:LEU:HA	1:7:A:LEU:HB2	1	0.11
(1,150)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	6	0.11
(1,150)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	6	0.11
(1,142)	1:12:A:LEU:H	1:13:A:LYS:H	9	0.11
(1,129)	1:14:A:GLN:HA	1:14:A:GLN:HG2	3	0.11
(1,109)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.11
(1,88)	1:24:A:PRO:HA	1:24:A:PRO:HB2	8	0.11
(1,75)	1:23:A:PRO:HG2	1:23:A:PRO:HG3	5	0.11
(1,75)	1:23:A:PRO:HG2	1:23:A:PRO:HG3	8	0.11
(1,14)	1:8:A:TYR:H	1:8:A:TYR:HA	5	0.11
(1,13)	1:12:A:LEU:H	1:12:A:LEU:HA	3	0.11
(1,13)	1:12:A:LEU:H	1:12:A:LEU:HA	4	0.11
(3,294)	1:9:A:ILE:HA	1:12:A:LEU:HB3	5	0.1
(3,265)	1:10:A:GLN:H	1:11:A:TRP:H	2	0.1
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.1
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.1
(3,171)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.1
(3,89)	1:24:A:PRO:HA	1:24:A:PRO:HD2	1	0.1
(2,308)	1:9:A:ILE:HA	1:12:A:LEU:HB3	5	0.1
(2,278)	1:10:A:GLN:H	1:11:A:TRP:H	2	0.1
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.1
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.1
(2,178)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.1
(2,92)	1:24:A:PRO:HA	1:24:A:PRO:HD2	1	0.1
(1,175)	1:9:A:ILE:H	1:9:A:ILE:HB	7	0.1
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	9	0.1
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	9	0.1
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	9	0.1
(1,155)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.1
(1,155)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.1
(1,155)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.1
(1,154)	1:7:A:LEU:HA	1:7:A:LEU:HB3	6	0.1
(1,152)	1:7:A:LEU:HA	1:7:A:LEU:HB2	3	0.1
(1,151)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	1	0.1
(1,151)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	1	0.1
(1,151)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	2	0.1
(1,151)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	2	0.1
(1,151)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	6	0.1
(1,151)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	6	0.1
(1,75)	1:23:A:PRO:HG2	1:23:A:PRO:HG3	1	0.1
(1,75)	1:23:A:PRO:HG2	1:23:A:PRO:HG3	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:23:A:PRO:HG2	1:23:A:PRO:HG3	3	0.1
(1,75)	1:23:A:PRO:HG2	1:23:A:PRO:HG3	4	0.1
(1,75)	1:23:A:PRO:HG2	1:23:A:PRO:HG3	6	0.1
(1,75)	1:23:A:PRO:HG2	1:23:A:PRO:HG3	7	0.1
(1,75)	1:23:A:PRO:HG2	1:23:A:PRO:HG3	9	0.1
(1,75)	1:23:A:PRO:HG2	1:23:A:PRO:HG3	10	0.1
(1,46)	1:21:A:ARG:HA	1:21:A:ARG:HG2	5	0.1
(1,46)	1:21:A:ARG:HA	1:21:A:ARG:HG3	5	0.1
(1,14)	1:8:A:TYR:H	1:8:A:TYR:HA	4	0.1
(1,14)	1:8:A:TYR:H	1:8:A:TYR:HA	8	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found