



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 05:11 PM UTC

PDB ID : 9GEB / pdb_00009geb
BMRB ID : 34951
Title : Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR) at 288K
Authors : Horvath, D.
Deposited on : 2024-08-07

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

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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

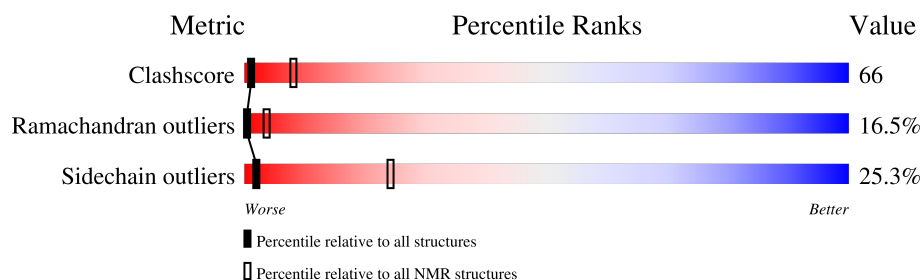
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 50%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	25	32% 36% 24% 8%

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:2-A:24 (23)	0.55	4

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

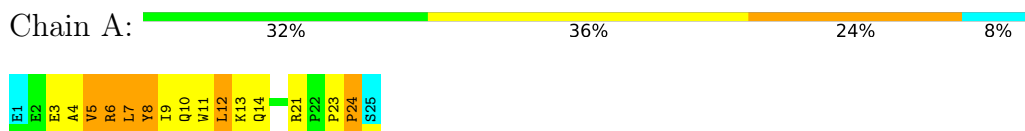
Mol	Chain	Residues	Atoms					Trace
1	A	25	Total	C	H	N	O	0
			390	124	193	35	38	

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)

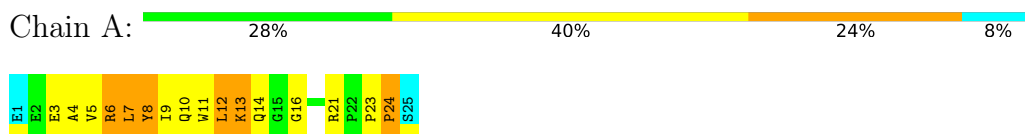


4.2 Scores per residue for each member of the ensemble

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

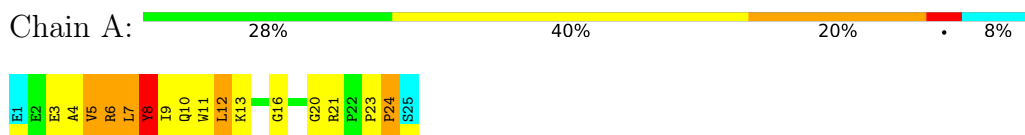
4.2.1 Score per residue for model 1

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



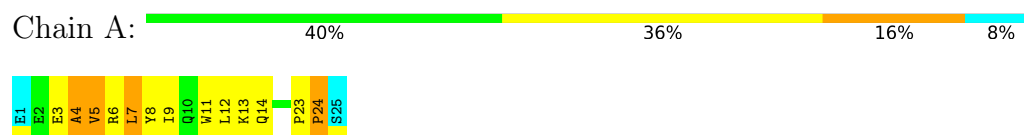
4.2.2 Score per residue for model 2

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



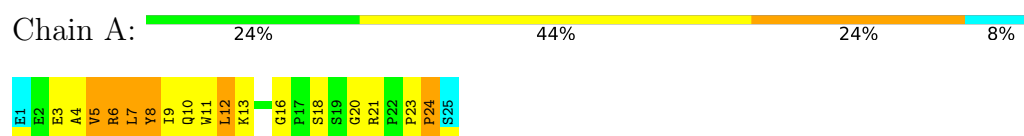
4.2.3 Score per residue for model 3

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



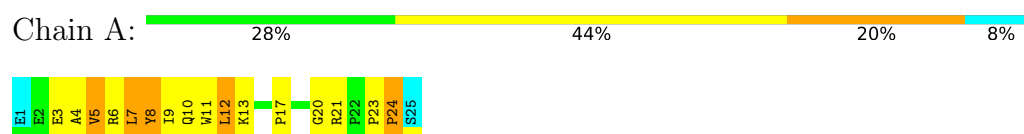
4.2.4 Score per residue for model 4 (medoid)

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



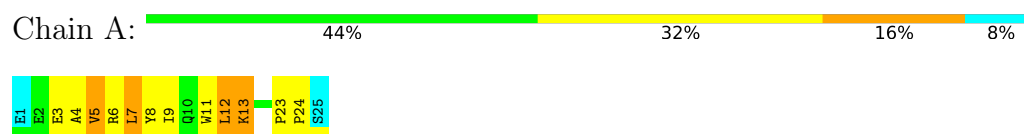
4.2.5 Score per residue for model 5

- 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)



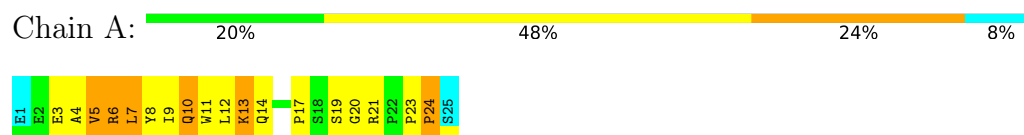
4.2.7 Score per residue for model 7

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



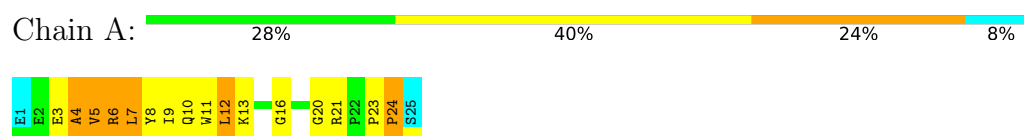
4.2.8 Score per residue for model 8

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



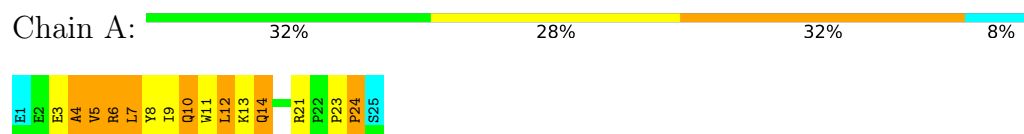
4.2.9 Score per residue for model 9

- 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	168
Number of shifts mapped to atoms	168
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	50%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.97±0.06	0±0/188 (0.0± 0.0%)	1.12±0.05	0±1/257 (0.1± 0.2%)
All	All	0.97	0/1880 (0.0%)	1.12	2/2570 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	1

There are no bond-length outliers.

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	6	ARG	CA-C-N	5.05	127.55	120.28	7	1
1	A	6	ARG	C-N-CA	5.05	127.55	120.28	7	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	8	TYR	Sidechain	1

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	181	180	180	24±2
All	All	1810	1800	1800	240

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 66.

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:HD13	1:A:24:PRO:HG2	0.97	1.35	8	9
1:A:8:TYR:CE2	1:A:12:LEU:HD21	0.92	2.00	2	8
1:A:8:TYR:O	1:A:11:TRP:HB3	0.81	1.75	7	10
1:A:11:TRP:CE3	1:A:12:LEU:HD23	0.80	2.12	10	10
1:A:6:ARG:HD2	1:A:7:LEU:N	0.76	1.96	5	3
1:A:7:LEU:HD13	1:A:24:PRO:HG3	0.73	1.60	6	4
1:A:7:LEU:HD13	1:A:24:PRO:CG	0.68	2.19	4	9
1:A:7:LEU:HD12	1:A:8:TYR:N	0.67	2.05	8	10
1:A:8:TYR:O	1:A:12:LEU:HG	0.66	1.90	3	10
1:A:3:GLU:O	1:A:6:ARG:HG3	0.66	1.90	6	3
1:A:8:TYR:CD2	1:A:12:LEU:HD21	0.63	2.28	2	5
1:A:3:GLU:HA	1:A:6:ARG:CG	0.63	2.24	7	3
1:A:3:GLU:O	1:A:7:LEU:HG	0.62	1.94	8	9
1:A:8:TYR:HE2	1:A:12:LEU:HD21	0.62	1.52	2	1
1:A:11:TRP:HE3	1:A:12:LEU:HD23	0.61	1.54	10	9
1:A:7:LEU:HD12	1:A:8:TYR:H	0.60	1.56	7	9
1:A:4:ALA:C	1:A:7:LEU:HD11	0.58	2.23	1	4
1:A:6:ARG:HD3	1:A:7:LEU:N	0.58	2.14	9	2
1:A:9:ILE:O	1:A:13:LYS:HE3	0.58	1.99	10	1
1:A:9:ILE:HA	1:A:12:LEU:CD1	0.57	2.29	7	10
1:A:9:ILE:HA	1:A:12:LEU:HG	0.57	1.75	7	10
1:A:5:VAL:N	1:A:7:LEU:HD11	0.57	2.15	10	9
1:A:3:GLU:C	1:A:5:VAL:H	0.56	2.09	10	10
1:A:10:GLN:O	1:A:14:GLN:HG2	0.56	2.00	10	1
1:A:5:VAL:O	1:A:9:ILE:HG13	0.55	2.01	7	8
1:A:8:TYR:HB2	1:A:24:PRO:CD	0.53	2.32	10	2
1:A:11:TRP:CZ3	1:A:12:LEU:HD23	0.53	2.38	8	2
1:A:8:TYR:C	1:A:8:TYR:CD2	0.52	2.87	7	1
1:A:11:TRP:HE1	1:A:21:ARG:C	0.51	2.13	9	7
1:A:8:TYR:CZ	1:A:12:LEU:HD21	0.51	2.40	8	4
1:A:9:ILE:HA	1:A:12:LEU:CG	0.50	2.36	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:TYR:CD2	1:A:8:TYR:C	0.50	2.89	2	4
1:A:9:ILE:HA	1:A:12:LEU:HD12	0.49	1.83	8	2
1:A:9:ILE:O	1:A:13:LYS:HD2	0.49	2.06	8	1
1:A:11:TRP:CH2	1:A:23:PRO:HG3	0.48	2.43	10	2
1:A:8:TYR:HB2	1:A:24:PRO:HD2	0.48	1.84	10	1
1:A:3:GLU:HA	1:A:6:ARG:HG3	0.48	1.86	7	1
1:A:10:GLN:HG3	1:A:11:TRP:N	0.48	2.24	8	1
1:A:5:VAL:HG22	1:A:9:ILE:HD11	0.47	1.85	7	2
1:A:9:ILE:O	1:A:13:LYS:HB2	0.47	2.09	3	2
1:A:11:TRP:CZ2	1:A:23:PRO:HG3	0.46	2.45	8	2
1:A:3:GLU:C	1:A:5:VAL:N	0.46	2.74	5	8
1:A:11:TRP:CE3	1:A:12:LEU:CD2	0.46	2.96	7	5
1:A:6:ARG:O	1:A:10:GLN:HB3	0.46	2.11	8	1
1:A:3:GLU:HA	1:A:6:ARG:HG2	0.45	1.87	7	3
1:A:21:ARG:NE	1:A:21:ARG:HA	0.45	2.26	2	1
1:A:5:VAL:HG13	1:A:6:ARG:N	0.44	2.28	10	5
1:A:9:ILE:O	1:A:13:LYS:HE2	0.44	2.13	3	2
1:A:12:LEU:HA	1:A:17:PRO:CD	0.44	2.42	8	1
1:A:5:VAL:C	1:A:7:LEU:HD12	0.42	2.39	7	1
1:A:7:LEU:CD1	1:A:8:TYR:N	0.41	2.80	8	2
1:A:13:LYS:N	1:A:13:LYS:HE2	0.41	2.30	1	1
1:A:12:LEU:HA	1:A:16:GLY:HA3	0.41	1.93	9	1
1:A:7:LEU:HB2	1:A:24:PRO:CB	0.41	2.45	6	1
1:A:6:ARG:CD	1:A:6:ARG:C	0.41	2.94	2	2
1:A:5:VAL:CG1	1:A:6:ARG:N	0.41	2.83	8	1
1:A:7:LEU:HD12	1:A:7:LEU:N	0.40	2.32	10	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	23/25 (92%)	14±2 (62±8%)	5±2 (22±7%)	4±1 (17±6%)	0	4
All	All	230/250 (92%)	142 (62%)	50 (22%)	38 (17%)	0	4

All 8 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	24	PRO	9
1	A	4	ALA	9
1	A	5	VAL	9
1	A	20	GLY	5
1	A	16	GLY	3
1	A	18	SER	1
1	A	17	PRO	1
1	A	19	SER	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	19/21 (90%)	14±1 (75±7%)	5±1 (25±7%)	2	24
All	All	190/210 (90%)	142 (75%)	48 (25%)	2	24

All 7 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	7	LEU	10
1	A	10	GLN	8
1	A	12	LEU	8
1	A	6	ARG	6
1	A	13	LYS	6
1	A	8	TYR	5
1	A	14	GLN	5

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 50% for the well-defined parts and 50% 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 [i](#)

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	168
Number of shifts mapped to atoms	168
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 [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 50%, i.e. 159 atoms were assigned a chemical shift out of a possible 315. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	44/110 (40%)	44/45 (98%)	0/46 (0%)	0/19 (0%)
Sidechain	105/184 (57%)	105/119 (88%)	0/56 (0%)	0/9 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	159/315 (50%)	159/174 (91%)	0/112 (0%)	0/29 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 168 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	47/120 (39%)	47/49 (96%)	0/50 (0%)	0/21 (0%)
Sidechain	111/194 (57%)	111/125 (89%)	0/60 (0%)	0/9 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	168/335 (50%)	168/184 (91%)	0/120 (0%)	0/31 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

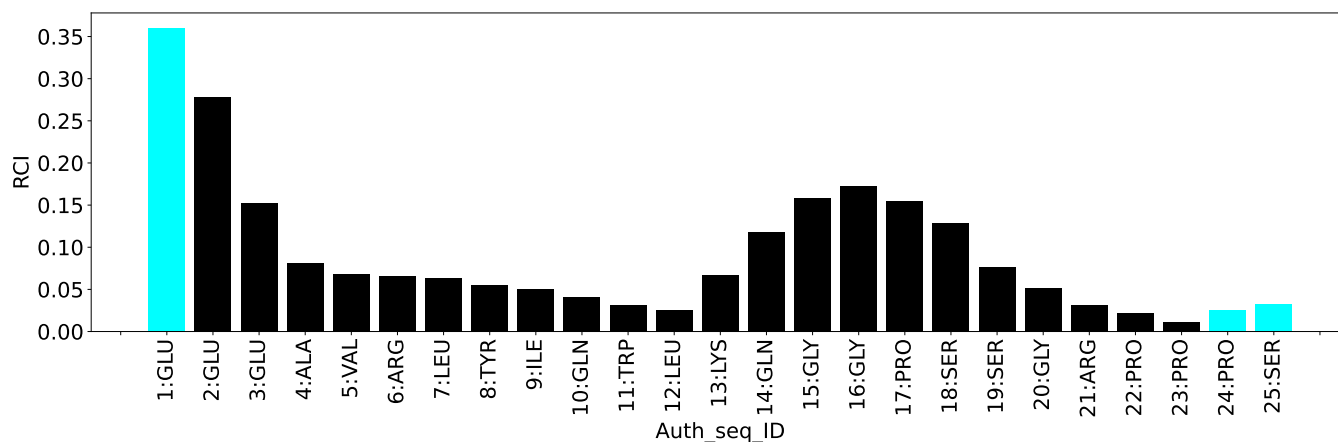
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	16	GLY	HA2	1.33	2.15 – 5.77	-7.3

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	1452
Intra-residue ($ i-j =0$)	816
Sequential ($ i-j =1$)	294
Medium range ($ i-j >1$ and $ i-j <5$)	180
Long range ($ i-j \geq 5$)	162
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	58.1
Number of long range restraints per residue ¹	6.5

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)	76.6	0.2
0.2-0.5 (Medium)	134.8	0.5
>0.5 (Large)	152.5	2.57

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 ⓘ

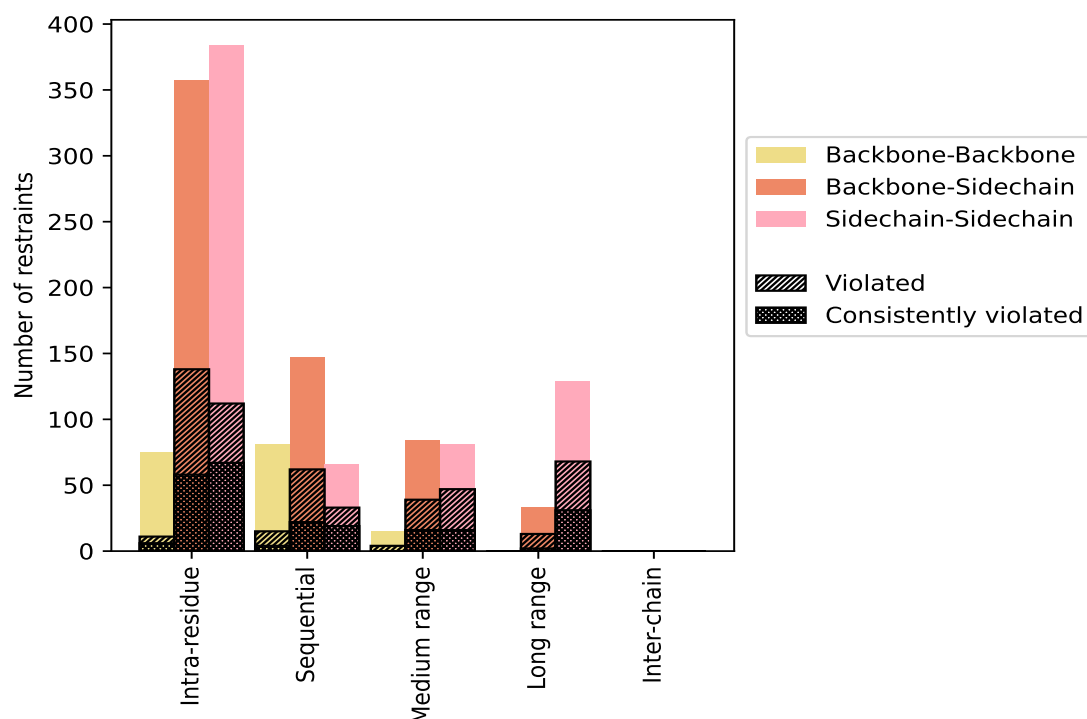
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	816	56.2	261	32.0	18.0	131	16.1	9.0
Backbone-Backbone	75	5.2	11	14.7	0.8	6	8.0	0.4
Backbone-Sidechain	357	24.6	138	38.7	9.5	58	16.2	4.0
Sidechain-Sidechain	384	26.4	112	29.2	7.7	67	17.4	4.6
Sequential ($i-j =1$)	294	20.2	110	37.4	7.6	45	15.3	3.1
Backbone-Backbone	81	5.6	15	18.5	1.0	4	4.9	0.3
Backbone-Sidechain	147	10.1	62	42.2	4.3	22	15.0	1.5
Sidechain-Sidechain	66	4.5	33	50.0	2.3	19	28.8	1.3
Medium range ($i-j >1$ & $i-j <5$)	180	12.4	90	50.0	6.2	32	17.8	2.2
Backbone-Backbone	15	1.0	4	26.7	0.3	0	0.0	0.0
Backbone-Sidechain	84	5.8	39	46.4	2.7	16	19.0	1.1
Sidechain-Sidechain	81	5.6	47	58.0	3.2	16	19.8	1.1
Long range ($i-j \geq 5$)	162	11.2	81	50.0	5.6	33	20.4	2.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	33	2.3	13	39.4	0.9	2	6.1	0.1
Sidechain-Sidechain	129	8.9	68	52.7	4.7	31	24.0	2.1
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	1452	100.0	542	37.3	37.3	241	16.6	16.6
Backbone-Backbone	171	11.8	30	17.5	2.1	10	5.8	0.7
Backbone-Sidechain	621	42.8	252	40.6	17.4	98	15.8	6.7
Sidechain-Sidechain	660	45.5	260	39.4	17.9	133	20.2	9.2

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

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



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

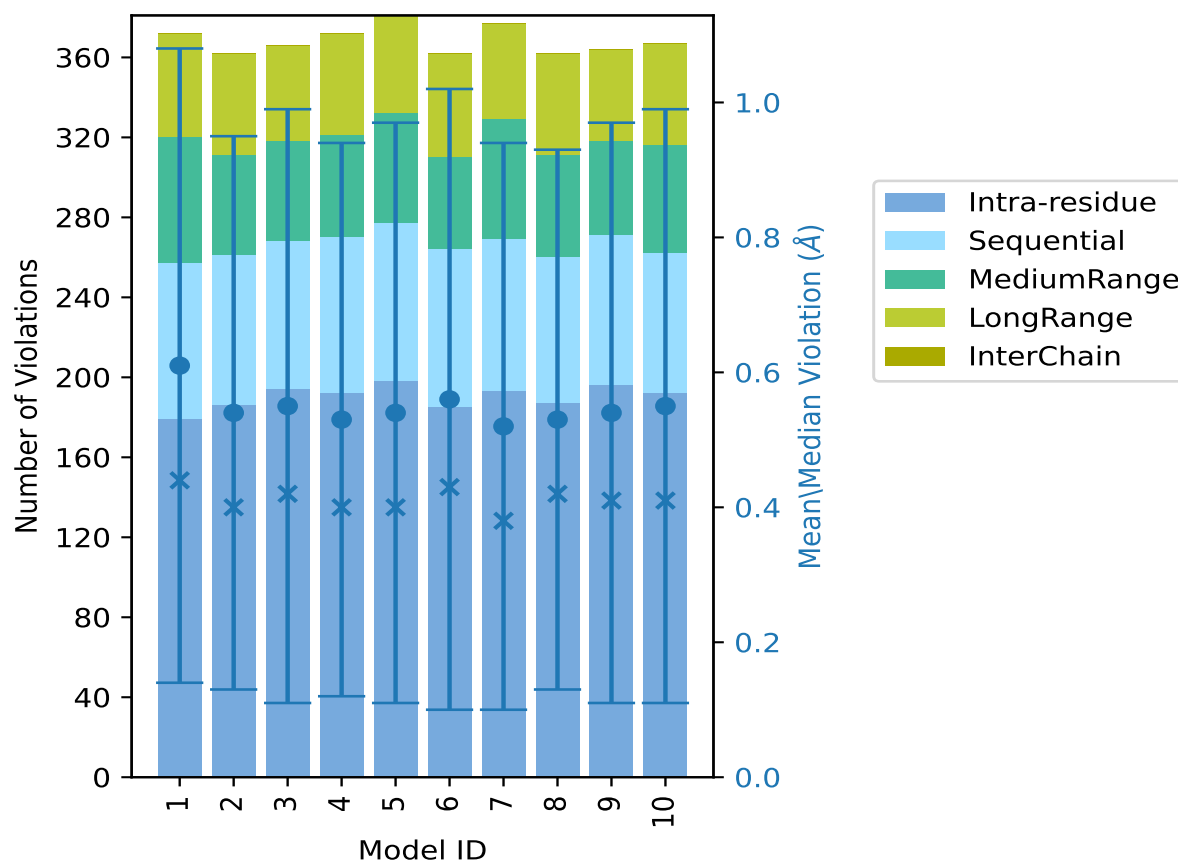
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	179	78	63	52	0	372	0.61	2.32	0.47	0.44
2	186	75	50	51	0	362	0.54	2.31	0.41	0.4
3	194	74	50	48	0	366	0.55	2.37	0.44	0.42
4	192	78	51	51	0	372	0.53	2.3	0.41	0.4
5	198	79	55	49	0	381	0.54	2.34	0.43	0.4
6	185	79	46	52	0	362	0.56	2.35	0.46	0.43
7	193	76	60	48	0	377	0.52	2.24	0.42	0.38
8	187	73	51	51	0	362	0.53	2.16	0.4	0.42
9	196	75	47	46	0	364	0.54	2.34	0.43	0.41
10	192	70	54	51	0	367	0.55	2.57	0.44	0.41

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, 910(IR:555, SQ:184, MR:90, LR:81, 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	%
26	12	17	19	0	74	1	10.0
19	11	6	1	0	37	2	20.0
16	5	8	7	0	36	3	30.0

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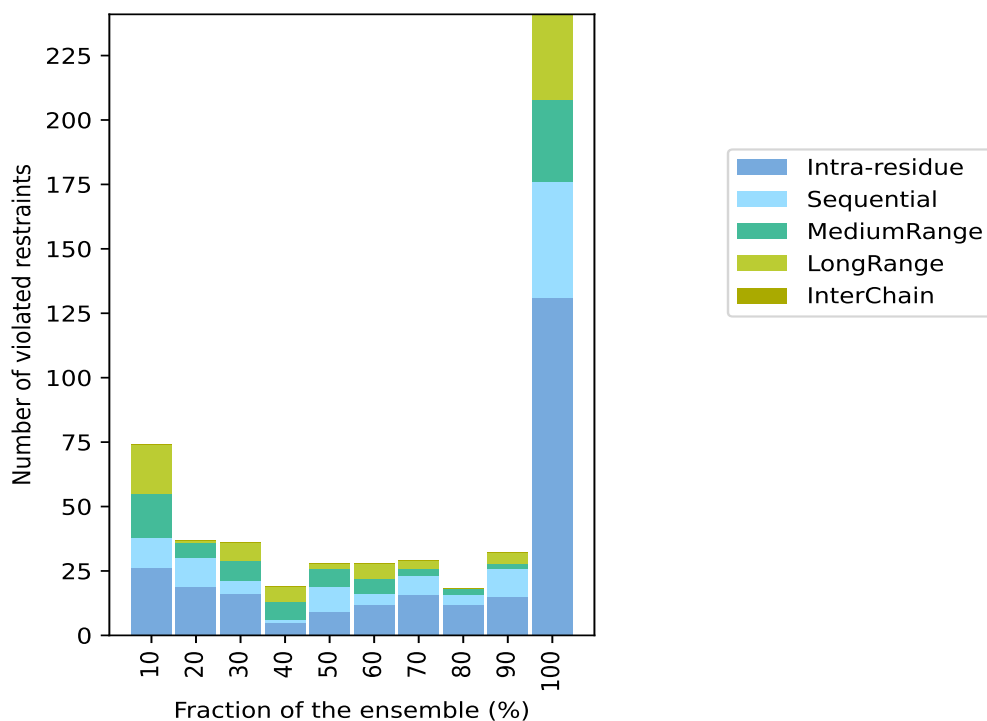
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
5	1	7	6	0	19	4	40.0
9	10	7	2	0	28	5	50.0
12	4	6	6	0	28	6	60.0
16	7	3	3	0	29	7	70.0
12	4	2	0	0	18	8	80.0
15	11	2	4	0	32	9	90.0
131	45	32	33	0	241	10	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](#)

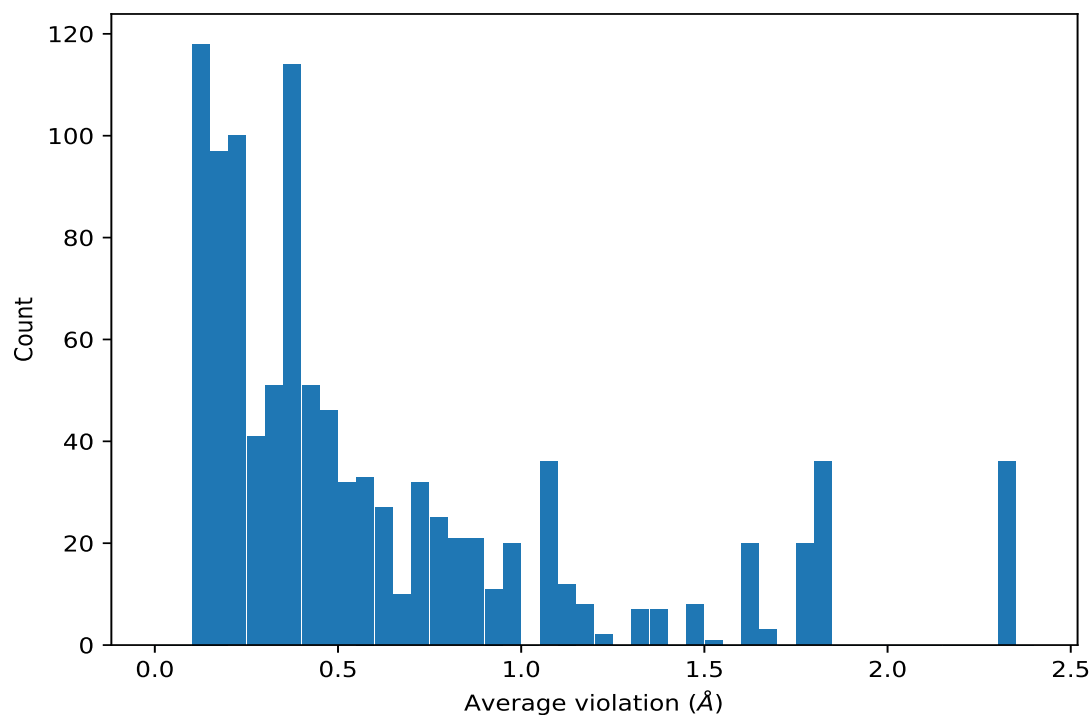


9.4 Most violated distance restraints in the ensemble [i](#)

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)
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	10	2.31	0.06	2.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	10	2.31	0.06	2.33
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	10	2.31	0.06	2.33
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	10	1.8	0.19	1.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	10	1.8	0.19	1.72
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	10	1.8	0.19	1.72
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	10	1.77	0.14	1.74
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	10	1.77	0.14	1.74
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	10	1.77	0.14	1.74
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	10	1.77	0.14	1.74
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	10	1.77	0.14	1.74
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	10	1.77	0.14	1.74
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	10	1.77	0.14	1.74
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	10	1.77	0.14	1.74
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	10	1.77	0.14	1.74
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	10	1.77	0.14	1.74
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	10	1.77	0.14	1.74
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	10	1.77	0.14	1.74
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	10	1.77	0.14	1.74
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	10	1.77	0.14	1.74
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	10	1.77	0.14	1.74
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	10	1.77	0.14	1.74
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	10	1.77	0.14	1.74
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	10	1.77	0.14	1.74
(2,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	10	1.76	0.26	1.76
(4,23)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	10	1.76	0.26	1.76
(1,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	10	1.69	0.04	1.69
(1,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	10	1.69	0.04	1.69
(1,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	10	1.69	0.04	1.69
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	10	1.62	0.06	1.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	10	1.62	0.06	1.64
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	10	1.62	0.06	1.64
(2,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	10	1.61	0.38	1.72
(4,32)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	10	1.61	0.38	1.72
(1,392)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	10	1.5	0.07	1.5
(2,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	10	1.48	0.64	1.72
(2,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	10	1.48	0.64	1.72
(4,33)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	10	1.48	0.64	1.72
(4,33)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	10	1.48	0.64	1.72
(2,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	10	1.47	0.43	1.6
(4,30)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	10	1.47	0.43	1.6
(1,237)	1:23:A:PRO:HA	1:23:A:PRO:HG3	10	1.39	0.02	1.39
(2,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	1.37	0.21	1.36
(2,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	1.37	0.21	1.36
(4,39)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	1.37	0.21	1.36
(4,39)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	1.37	0.21	1.36
(2,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	1.36	0.06	1.36
(3,281)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	1.36	0.06	1.36
(1,396)	1:12:A:LEU:HD21	1:17:A:PRO:HD3	10	1.34	0.18	1.45
(1,396)	1:12:A:LEU:HD22	1:17:A:PRO:HD3	10	1.34	0.18	1.45
(1,396)	1:12:A:LEU:HD23	1:17:A:PRO:HD3	10	1.34	0.18	1.45
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	10	1.31	0.44	1.38
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	10	1.31	0.44	1.38
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	10	1.31	0.44	1.38
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	10	1.31	0.44	1.38
(2,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.2	0.08	1.2
(3,280)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.2	0.08	1.2
(2,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	1.16	0.06	1.18
(3,383)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	1.16	0.06	1.18
(2,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	10	1.11	0.44	0.98

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	10	1.11	0.44	0.98
(2,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	10	1.11	0.44	0.98
(3,370)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	10	1.11	0.44	0.98
(3,370)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	10	1.11	0.44	0.98
(3,370)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	10	1.11	0.44	0.98
(1,404)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	10	1.1	0.11	1.12
(1,404)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	10	1.1	0.11	1.12
(1,404)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	10	1.1	0.11	1.12
(1,367)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	10	1.1	0.33	1.25
(1,367)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	10	1.1	0.33	1.25
(2,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	10	1.09	0.63	1.06
(3,360)	1:15:A:GLY:HA3	1:18:A:SER:HB3	10	1.09	0.63	1.06
(1,318)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	10	1.09	0.14	1.06
(1,330)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	10	1.09	0.12	1.12
(1,330)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	10	1.09	0.12	1.12
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	10	1.08	0.19	1.0
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	10	1.08	0.19	1.0
(1,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	10	1.06	0.26	1.06
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	10	1.05	0.14	1.02
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	10	1.05	0.14	1.02
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	10	1.05	0.14	1.02
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	10	1.05	0.14	1.02
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	10	1.05	0.14	1.02
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	10	1.05	0.14	1.02
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	10	1.05	0.14	1.02
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	10	1.05	0.14	1.02

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	10	1.05	0.14	1.02
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	0.99	0.14	1.02
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	0.99	0.14	1.02
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	0.99	0.14	1.02
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	0.99	0.14	1.02
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	0.99	0.14	1.02
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	0.99	0.14	1.02
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	10	0.98	0.19	1.04
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	10	0.98	0.19	1.04
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	10	0.98	0.19	1.04
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	10	0.98	0.19	1.04
(2,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.96	0.02	0.96
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.96	0.02	0.96
(1,32)	1:3:A:GLU:H	1:4:A:ALA:H	10	0.95	0.13	0.98
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.92	0.02	0.92
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.92	0.02	0.92
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.92	0.02	0.92
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.92	0.02	0.92
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.92	0.02	0.92
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.92	0.02	0.92
(1,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	10	0.91	0.38	1.02
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.9	0.01	0.9
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.89	0.03	0.89
(2,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	10	0.88	0.13	0.94
(3,421)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	10	0.88	0.13	0.94
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	10	0.86	0.13	0.8
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	10	0.86	0.13	0.8
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	10	0.86	0.13	0.8
(1,54)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.85	0.12	0.9
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG2	10	0.85	0.08	0.83
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG2	10	0.85	0.08	0.83
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG2	10	0.85	0.08	0.83
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG3	10	0.85	0.08	0.83
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG3	10	0.85	0.08	0.83
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG3	10	0.85	0.08	0.83
(2,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	10	0.85	0.47	0.73
(3,382)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	10	0.85	0.47	0.73
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	10	0.82	0.17	0.9
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	10	0.82	0.17	0.9
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	10	0.82	0.17	0.9
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	10	0.82	0.17	0.9
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	10	0.82	0.17	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	10	0.82	0.17	0.9
(1,332)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.82	0.04	0.84
(2,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	10	0.82	0.14	0.8
(2,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	10	0.82	0.14	0.8
(2,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	10	0.82	0.14	0.8
(4,29)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	10	0.82	0.14	0.8
(4,29)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	10	0.82	0.14	0.8
(4,29)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	10	0.82	0.14	0.8
(2,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.81	0.01	0.82
(3,134)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.81	0.01	0.82
(1,45)	1:5:A:VAL:H	1:6:A:ARG:H	10	0.79	0.06	0.79
(1,465)	1:3:A:GLU:HA	1:6:A:ARG:HB3	10	0.78	0.31	0.83
(2,92)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.78	0.01	0.77
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.78	0.01	0.77
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.77	0.04	0.78
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.77	0.04	0.78
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.77	0.04	0.78
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.77	0.04	0.78
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.77	0.04	0.78
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.77	0.04	0.78
(1,239)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	10	0.77	0.01	0.77
(1,408)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	10	0.77	0.14	0.78
(2,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	10	0.76	0.15	0.86
(3,364)	1:9:A:ILE:HA	1:12:A:LEU:HB3	10	0.76	0.15	0.86
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD11	10	0.76	0.08	0.78
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD12	10	0.76	0.08	0.78
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD13	10	0.76	0.08	0.78
(2,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	10	0.74	0.27	0.74
(3,394)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	10	0.74	0.27	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.73	0.02	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.73	0.02	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.73	0.02	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.73	0.02	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.73	0.02	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.73	0.02	0.74
(1,117)	1:9:A:ILE:H	1:9:A:ILE:HG13	10	0.73	0.05	0.72
(2,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.72	0.34	0.88
(3,70)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.72	0.34	0.88
(2,306)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	10	0.72	0.06	0.74
(3,286)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	10	0.72	0.06	0.74
(1,326)	1:11:A:TRP:HB3	1:12:A:LEU:H	10	0.7	0.03	0.71
(1,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	0.7	0.21	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	0.7	0.21	0.69
(2,304)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.7	0.03	0.69
(3,285)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.7	0.03	0.69
(1,173)	1:6:A:ARG:HD2	1:7:A:LEU:H	10	0.68	0.37	0.54
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	10	0.67	0.04	0.68
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	10	0.67	0.04	0.68
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	10	0.67	0.04	0.68
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	0.64	0.04	0.62
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	10	0.64	0.04	0.62
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	10	0.64	0.04	0.62
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	10	0.64	0.04	0.62
(1,258)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.64	0.04	0.64
(1,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.64	0.06	0.64
(1,235)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.64	0.01	0.64
(1,102)	1:9:A:ILE:HA	1:9:A:ILE:HG12	10	0.64	0.03	0.63
(2,472)	1:13:A:LYS:H	1:14:A:GLN:HA	10	0.62	0.17	0.54
(4,41)	1:13:A:LYS:H	1:14:A:GLN:HA	10	0.62	0.17	0.54
(1,154)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.61	0.0	0.61
(1,305)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	0.6	0.02	0.61
(1,28)	1:3:A:GLU:HB3	1:4:A:ALA:H	10	0.6	0.16	0.6
(2,201)	1:17:A:PRO:HA	1:17:A:PRO:HD3	10	0.6	0.06	0.62
(4,15)	1:17:A:PRO:HA	1:17:A:PRO:HD3	10	0.6	0.06	0.62
(1,319)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	10	0.59	0.21	0.54
(1,194)	1:18:A:SER:H	1:18:A:SER:HB2	10	0.59	0.16	0.62
(1,194)	1:18:A:SER:H	1:18:A:SER:HB3	10	0.59	0.16	0.62
(1,12)	1:18:A:SER:H	1:18:A:SER:HA	10	0.57	0.04	0.55
(2,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	10	0.57	0.24	0.42
(2,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	10	0.57	0.24	0.42
(2,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	10	0.57	0.24	0.42
(4,28)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	10	0.57	0.24	0.42
(4,28)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	10	0.57	0.24	0.42
(4,28)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	10	0.57	0.24	0.42
(1,158)	1:12:A:LEU:HA	1:12:A:LEU:HB3	10	0.55	0.03	0.56
(2,389)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.55	0.15	0.6
(3,363)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.55	0.15	0.6
(1,50)	1:6:A:ARG:HA	1:6:A:ARG:HB2	10	0.55	0.09	0.59
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	0.55	0.02	0.55
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	0.55	0.02	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	10	0.55	0.02	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	10	0.55	0.02	0.55
(1,218)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.55	0.02	0.54
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.54	0.08	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	10	0.54	0.08	0.52
(2,303)	1:11:A:TRP:HA	1:11:A:TRP:HE3	10	0.54	0.08	0.58
(4,19)	1:11:A:TRP:HA	1:11:A:TRP:HE3	10	0.54	0.08	0.58
(1,243)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.54	0.0	0.54
(1,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.54	0.08	0.54
(1,388)	1:5:A:VAL:HA	1:8:A:TYR:HB3	10	0.54	0.12	0.52
(2,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	10	0.53	0.2	0.52
(3,381)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	10	0.53	0.2	0.52
(1,240)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	10	0.52	0.0	0.52
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	10	0.51	0.02	0.52
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	10	0.51	0.02	0.52
(1,444)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	10	0.51	0.13	0.52
(1,444)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	10	0.51	0.13	0.52
(1,444)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	10	0.51	0.13	0.52
(1,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	10	0.51	0.13	0.52
(1,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	10	0.51	0.13	0.52
(1,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	10	0.51	0.13	0.52
(2,116)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.51	0.02	0.51
(3,106)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.51	0.02	0.51
(1,209)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	10	0.49	0.06	0.49
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG2	10	0.49	0.05	0.49
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG3	10	0.49	0.05	0.49
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB2	10	0.48	0.08	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB3	10	0.48	0.08	0.53
(1,10)	1:15:A:GLY:H	1:15:A:GLY:HA2	10	0.47	0.05	0.48
(1,107)	1:9:A:ILE:HB	1:9:A:ILE:HG13	10	0.47	0.01	0.47
(1,385)	1:7:A:LEU:HD11	1:8:A:TYR:HA	10	0.47	0.05	0.46
(1,385)	1:7:A:LEU:HD12	1:8:A:TYR:HA	10	0.47	0.05	0.46
(1,385)	1:7:A:LEU:HD13	1:8:A:TYR:HA	10	0.47	0.05	0.46
(1,261)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.46	0.03	0.46
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.45	0.04	0.44
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.45	0.04	0.44
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.45	0.04	0.44
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.45	0.04	0.44
(1,213)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.44	0.0	0.44
(1,314)	1:8:A:TYR:HD1	1:9:A:ILE:H	10	0.44	0.15	0.42
(1,314)	1:8:A:TYR:HD2	1:9:A:ILE:H	10	0.44	0.15	0.42
(1,231)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.44	0.0	0.44
(1,231)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	10	0.44	0.0	0.44
(2,325)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.44	0.08	0.44
(4,21)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.44	0.08	0.44
(1,166)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.43	0.01	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,166)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.43	0.01	0.43
(1,166)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.43	0.01	0.43
(1,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.43	0.06	0.46
(1,192)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.41	0.0	0.41
(1,338)	1:21:A:ARG:H	1:21:A:ARG:HB2	10	0.41	0.13	0.38
(1,254)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.41	0.07	0.39
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	10	0.4	0.0	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	10	0.4	0.0	0.4
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD2	10	0.39	0.03	0.4
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.39	0.03	0.4
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.39	0.01	0.38
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	10	0.39	0.01	0.38
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.38	0.53	0.2
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.38	0.53	0.2
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.38	0.53	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.38	0.53	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.38	0.53	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.38	0.53	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.38	0.53	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.38	0.53	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.38	0.53	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.38	0.53	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.38	0.53	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.38	0.53	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.38	0.53	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.38	0.53	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.38	0.53	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.38	0.53	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.38	0.53	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.38	0.53	0.2
(1,238)	1:23:A:PRO:HA	1:23:A:PRO:HG2	10	0.38	0.01	0.38
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	10	0.38	0.03	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	10	0.38	0.03	0.38
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	10	0.38	0.03	0.38
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	10	0.38	0.03	0.38
(2,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	10	0.37	0.22	0.32
(4,31)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	10	0.37	0.22	0.32
(1,278)	1:21:A:ARG:HA	1:21:A:ARG:HB3	10	0.37	0.05	0.38
(1,167)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.37	0.01	0.37
(1,167)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.37	0.01	0.37
(1,167)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.37	0.01	0.37
(1,7)	1:19:A:SER:H	1:19:A:SER:HA	10	0.37	0.31	0.18
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	10	0.37	0.1	0.4
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB3	10	0.37	0.1	0.4
(1,79)	1:7:A:LEU:HA	1:7:A:LEU:HB3	10	0.36	0.01	0.37
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	10	0.36	0.02	0.37
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.36	0.02	0.37
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	10	0.36	0.03	0.36
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	10	0.36	0.03	0.36
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	10	0.36	0.03	0.36
(1,217)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.36	0.0	0.36
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	10	0.35	0.05	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	10	0.35	0.05	0.36
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	10	0.35	0.05	0.36
(1,56)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	10	0.35	0.15	0.29
(1,18)	1:3:A:GLU:HA	1:3:A:GLU:HB2	10	0.34	0.02	0.34
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.34	0.03	0.35
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.34	0.03	0.35
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.34	0.03	0.35
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.34	0.03	0.35
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.34	0.03	0.36
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.34	0.03	0.36
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.34	0.03	0.36
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.34	0.03	0.36
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.34	0.03	0.36
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.34	0.03	0.36
(1,143)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.34	0.0	0.34
(1,232)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	10	0.34	0.01	0.34
(1,232)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.34	0.01	0.34
(2,139)	1:11:A:TRP:H	1:11:A:TRP:HD1	10	0.34	0.03	0.34
(4,13)	1:11:A:TRP:H	1:11:A:TRP:HD1	10	0.34	0.03	0.34
(2,340)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.32	0.05	0.32
(3,318)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.32	0.05	0.32
(1,381)	1:6:A:ARG:HA	1:9:A:ILE:HB	10	0.32	0.12	0.36
(1,63)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.32	0.0	0.32
(2,315)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.31	0.02	0.31
(3,295)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.31	0.02	0.31
(1,263)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	10	0.3	0.02	0.3
(1,420)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	10	0.3	0.13	0.23
(1,420)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	10	0.3	0.13	0.23
(1,85)	1:7:A:LEU:HD11	1:7:A:LEU:HG	10	0.3	0.01	0.3
(1,85)	1:7:A:LEU:HD12	1:7:A:LEU:HG	10	0.3	0.01	0.3
(1,85)	1:7:A:LEU:HD13	1:7:A:LEU:HG	10	0.3	0.01	0.3
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.3	0.01	0.3
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	10	0.3	0.01	0.3
(1,96)	1:8:A:TYR:HA	1:8:A:TYR:HB2	10	0.29	0.03	0.29
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.29	0.1	0.29
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	10	0.29	0.1	0.29
(2,461)	1:3:A:GLU:HG2	1:6:A:ARG:H	10	0.29	0.04	0.26
(2,461)	1:3:A:GLU:HG3	1:6:A:ARG:H	10	0.29	0.04	0.26
(4,40)	1:3:A:GLU:HG2	1:6:A:ARG:H	10	0.29	0.04	0.26
(4,40)	1:3:A:GLU:HG3	1:6:A:ARG:H	10	0.29	0.04	0.26
(1,267)	1:24:A:PRO:HA	1:24:A:PRO:HB3	10	0.27	0.02	0.27
(1,419)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	10	0.27	0.0	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,285)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	10	0.26	0.0	0.26
(1,81)	1:7:A:LEU:HB3	1:7:A:LEU:HG	10	0.26	0.02	0.26
(1,241)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.26	0.01	0.26
(2,48)	1:6:A:ARG:HA	1:6:A:ARG:HD2	10	0.26	0.08	0.25
(4,3)	1:6:A:ARG:HA	1:6:A:ARG:HD2	10	0.26	0.08	0.25
(1,273)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	10	0.25	0.0	0.25
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.25	0.02	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.25	0.02	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.25	0.02	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.25	0.02	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.25	0.02	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.25	0.02	0.26
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD11	10	0.24	0.04	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD12	10	0.24	0.04	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD13	10	0.24	0.04	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	10	0.24	0.04	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	10	0.24	0.04	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	10	0.24	0.04	0.25
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	10	0.24	0.03	0.25
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB3	10	0.24	0.03	0.25
(1,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.24	0.02	0.23
(1,99)	1:8:A:TYR:H	1:8:A:TYR:HB3	10	0.24	0.02	0.24
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	10	0.23	0.03	0.24
(1,84)	1:7:A:LEU:HD21	1:7:A:LEU:HG	10	0.23	0.01	0.22
(1,84)	1:7:A:LEU:HD22	1:7:A:LEU:HG	10	0.23	0.01	0.22
(1,84)	1:7:A:LEU:HD23	1:7:A:LEU:HG	10	0.23	0.01	0.22
(1,123)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	10	0.22	0.01	0.22
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	10	0.22	0.02	0.22
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	10	0.22	0.02	0.22
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	10	0.22	0.02	0.22
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	10	0.22	0.02	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	10	0.21	0.02	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	10	0.21	0.02	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	10	0.21	0.02	0.22
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD21	10	0.21	0.02	0.22
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD22	10	0.21	0.02	0.22
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD23	10	0.21	0.02	0.22
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD21	10	0.21	0.02	0.22
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD22	10	0.21	0.02	0.22
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD23	10	0.21	0.02	0.22
(1,250)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	10	0.21	0.01	0.21
(2,335)	1:7:A:LEU:HB3	1:8:A:TYR:H	10	0.21	0.02	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,314)	1:7:A:LEU:HB3	1:8:A:TYR:H	10	0.21	0.02	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG11	10	0.21	0.02	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG12	10	0.21	0.02	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG13	10	0.21	0.02	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG21	10	0.21	0.02	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG22	10	0.21	0.02	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG23	10	0.21	0.02	0.21
(1,195)	1:19:A:SER:HB2	1:19:A:SER:HB3	10	0.2	0.01	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.2	0.02	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.2	0.02	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.2	0.02	0.2
(1,205)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.19	0.0	0.19
(1,236)	1:23:A:PRO:HA	1:23:A:PRO:HB2	10	0.19	0.0	0.19
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	10	0.19	0.01	0.18
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	10	0.19	0.01	0.18
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG21	10	0.18	0.04	0.17
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG22	10	0.18	0.04	0.17
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG23	10	0.18	0.04	0.17
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG21	10	0.18	0.04	0.17
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG22	10	0.18	0.04	0.17
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG23	10	0.18	0.04	0.17
(1,156)	1:12:A:LEU:HA	1:12:A:LEU:HB2	10	0.18	0.03	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.18	0.01	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.18	0.01	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.18	0.01	0.18
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	10	0.18	0.04	0.17
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	10	0.18	0.04	0.17
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	10	0.18	0.04	0.17
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	10	0.18	0.04	0.17
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	10	0.18	0.04	0.17
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	10	0.18	0.04	0.17
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.18	0.01	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.18	0.01	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.18	0.01	0.18
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	10	0.18	0.04	0.17
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	10	0.18	0.04	0.17
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	10	0.18	0.04	0.17
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	10	0.18	0.04	0.17
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	10	0.18	0.04	0.17
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	10	0.18	0.04	0.17
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.17	0.01	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.17	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.17	0.01	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.17	0.01	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.17	0.01	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.17	0.01	0.16
(1,124)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	10	0.16	0.0	0.16
(2,106)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.15	0.01	0.15
(3,96)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.15	0.01	0.15
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	10	0.14	0.0	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	10	0.14	0.0	0.14
(1,162)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.14	0.01	0.14
(1,110)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	10	0.14	0.01	0.14
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.13	0.02	0.13
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.13	0.02	0.13
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.13	0.02	0.13
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.13	0.02	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG21	10	0.12	0.0	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG22	10	0.12	0.0	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG23	10	0.12	0.0	0.12
(1,253)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	10	0.12	0.01	0.12
(1,226)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	10	0.12	0.0	0.12
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB1	10	0.11	0.0	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB2	10	0.11	0.0	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB3	10	0.11	0.0	0.11
(1,80)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.11	0.0	0.11
(1,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	9	1.19	0.12	1.23
(1,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	9	1.19	0.12	1.23
(1,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	9	1.19	0.12	1.23
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG11	9	0.96	0.17	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG12	9	0.96	0.17	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG13	9	0.96	0.17	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG21	9	0.96	0.17	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG22	9	0.96	0.17	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG23	9	0.96	0.17	1.01
(1,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	9	0.9	0.26	1.03
(1,47)	1:5:A:VAL:HG11	1:6:A:ARG:H	9	0.89	0.05	0.9
(1,47)	1:5:A:VAL:HG12	1:6:A:ARG:H	9	0.89	0.05	0.9
(1,47)	1:5:A:VAL:HG13	1:6:A:ARG:H	9	0.89	0.05	0.9
(1,47)	1:5:A:VAL:HG21	1:6:A:ARG:H	9	0.89	0.05	0.9
(1,47)	1:5:A:VAL:HG22	1:6:A:ARG:H	9	0.89	0.05	0.9
(1,47)	1:5:A:VAL:HG23	1:6:A:ARG:H	9	0.89	0.05	0.9
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	9	0.72	0.26	0.88
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	9	0.72	0.26	0.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	9	0.72	0.26	0.88
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	9	0.72	0.26	0.88
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	9	0.72	0.26	0.88
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	9	0.72	0.26	0.88
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG2	9	0.69	0.11	0.74
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG3	9	0.69	0.11	0.74
(1,347)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	9	0.67	0.21	0.75
(1,34)	1:5:A:VAL:HA	1:5:A:VAL:HB	9	0.57	0.01	0.58
(2,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	9	0.56	0.2	0.46
(3,168)	1:13:A:LYS:H	1:13:A:LYS:HB3	9	0.56	0.2	0.46
(1,270)	1:24:A:PRO:HA	1:24:A:PRO:HG3	9	0.53	0.07	0.52
(1,256)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	9	0.52	0.09	0.5
(1,430)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	9	0.47	0.11	0.47
(1,430)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	9	0.47	0.11	0.47
(1,430)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	9	0.47	0.11	0.47
(2,46)	1:5:A:VAL:HB	1:6:A:ARG:H	9	0.45	0.01	0.46
(3,44)	1:5:A:VAL:HB	1:6:A:ARG:H	9	0.45	0.01	0.46
(1,327)	1:8:A:TYR:HB3	1:9:A:ILE:H	9	0.39	0.07	0.37
(2,264)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	9	0.38	0.01	0.38
(3,247)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	9	0.38	0.01	0.38
(1,153)	1:16:A:GLY:H	1:16:A:GLY:HA3	9	0.37	0.01	0.38
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG11	9	0.37	0.06	0.36
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG12	9	0.37	0.06	0.36
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG13	9	0.37	0.06	0.36
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG21	9	0.37	0.06	0.36
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG22	9	0.37	0.06	0.36
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG23	9	0.37	0.06	0.36
(1,468)	1:5:A:VAL:HG11	1:6:A:ARG:HA	9	0.37	0.03	0.36
(1,468)	1:5:A:VAL:HG12	1:6:A:ARG:HA	9	0.37	0.03	0.36
(1,468)	1:5:A:VAL:HG13	1:6:A:ARG:HA	9	0.37	0.03	0.36
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:HA	9	0.37	0.03	0.36
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:HA	9	0.37	0.03	0.36
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:HA	9	0.37	0.03	0.36
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	9	0.33	0.08	0.35
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	9	0.33	0.08	0.35
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	9	0.33	0.08	0.35
(1,376)	1:8:A:TYR:HA	1:24:A:PRO:HD3	9	0.29	0.12	0.29
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG2	9	0.24	0.06	0.23
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG3	9	0.24	0.06	0.23
(1,30)	1:4:A:ALA:HA	1:5:A:VAL:H	9	0.22	0.03	0.22
(2,36)	1:5:A:VAL:H	1:5:A:VAL:HB	9	0.19	0.02	0.19
(3,35)	1:5:A:VAL:H	1:5:A:VAL:HB	9	0.19	0.02	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,384)	1:7:A:LEU:HD11	1:8:A:TYR:HA	9	0.18	0.05	0.16
(1,384)	1:7:A:LEU:HD12	1:8:A:TYR:HA	9	0.18	0.05	0.16
(1,384)	1:7:A:LEU:HD13	1:8:A:TYR:HA	9	0.18	0.05	0.16
(1,144)	1:11:A:TRP:H	1:11:A:TRP:HB2	9	0.15	0.03	0.14
(1,260)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	9	0.14	0.02	0.15
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB1	9	0.14	0.01	0.14
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB2	9	0.14	0.01	0.14
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB3	9	0.14	0.01	0.14
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	8	0.91	0.04	0.9
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD2	8	0.82	0.26	0.88
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD3	8	0.82	0.26	0.88
(2,339)	1:10:A:GLN:HB2	1:11:A:TRP:H	8	0.77	0.03	0.78
(3,317)	1:10:A:GLN:HB2	1:11:A:TRP:H	8	0.77	0.03	0.78
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	8	0.76	0.32	0.9
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	8	0.76	0.32	0.9
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	8	0.76	0.32	0.9
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	8	0.76	0.32	0.9
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	8	0.76	0.32	0.9
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	8	0.76	0.32	0.9
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	8	0.63	0.05	0.62
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	8	0.63	0.05	0.62
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	8	0.63	0.05	0.62
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	8	0.63	0.05	0.62
(1,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	8	0.55	0.33	0.56
(1,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	8	0.55	0.33	0.56
(1,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	8	0.55	0.33	0.56
(1,284)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	8	0.41	0.05	0.4
(2,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	8	0.38	0.15	0.34
(3,114)	1:10:A:GLN:H	1:10:A:GLN:HB2	8	0.38	0.15	0.34
(1,288)	1:13:A:LYS:H	1:14:A:GLN:H	8	0.34	0.11	0.38
(1,283)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	8	0.3	0.05	0.33
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB2	8	0.25	0.01	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB3	8	0.25	0.01	0.25
(1,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	8	0.25	0.06	0.27
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG21	8	0.16	0.02	0.15
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG22	8	0.16	0.02	0.15
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG23	8	0.16	0.02	0.15
(2,22)	1:3:A:GLU:H	1:3:A:GLU:HB2	8	0.12	0.02	0.12
(3,21)	1:3:A:GLU:H	1:3:A:GLU:HB2	8	0.12	0.02	0.12
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE2	7	1.16	0.4	1.35
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE3	7	1.16	0.4	1.35
(1,58)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	7	1.1	0.08	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	7	1.06	0.39	1.29
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	7	0.73	0.36	0.94
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	7	0.73	0.36	0.94
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	7	0.73	0.36	0.94
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	7	0.73	0.36	0.94
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	7	0.73	0.36	0.94
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	7	0.73	0.36	0.94
(1,356)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	7	0.67	0.24	0.71
(2,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	7	0.61	0.02	0.62
(3,173)	1:14:A:GLN:H	1:14:A:GLN:HB2	7	0.61	0.02	0.62
(1,416)	1:8:A:TYR:HB2	1:24:A:PRO:HD2	7	0.58	0.29	0.68
(1,341)	1:21:A:ARG:H	1:21:A:ARG:HG2	7	0.57	0.16	0.61
(1,69)	1:6:A:ARG:H	1:6:A:ARG:HB3	7	0.51	0.1	0.56
(2,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	7	0.48	0.13	0.42
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HG3	7	0.48	0.13	0.42
(2,333)	1:12:A:LEU:HB3	1:13:A:LYS:H	7	0.42	0.11	0.48
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	7	0.42	0.11	0.48
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB2	7	0.41	0.01	0.4
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB3	7	0.41	0.01	0.4
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG11	7	0.4	0.59	0.16
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG12	7	0.4	0.59	0.16
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG13	7	0.4	0.59	0.16
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG11	7	0.4	0.59	0.16
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG12	7	0.4	0.59	0.16
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG13	7	0.4	0.59	0.16
(1,431)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	7	0.39	0.32	0.26
(1,431)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	7	0.39	0.32	0.26
(1,431)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	7	0.39	0.32	0.26
(2,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	7	0.34	0.11	0.31
(3,176)	1:14:A:GLN:HA	1:14:A:GLN:HG2	7	0.34	0.11	0.31
(1,344)	1:14:A:GLN:HE21	1:14:A:GLN:HG3	7	0.33	0.28	0.17
(1,150)	1:15:A:GLY:HA2	1:16:A:GLY:H	7	0.27	0.11	0.27
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD21	7	0.24	0.08	0.24
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD22	7	0.24	0.08	0.24
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD23	7	0.24	0.08	0.24
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	7	0.23	0.02	0.23
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	7	0.23	0.02	0.23
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	7	0.23	0.02	0.23
(2,349)	1:24:A:PRO:HB3	1:25:A:SER:H	7	0.22	0.12	0.2
(3,327)	1:24:A:PRO:HB3	1:25:A:SER:H	7	0.22	0.12	0.2
(2,129)	1:10:A:GLN:H	1:10:A:GLN:HG2	7	0.16	0.01	0.16
(3,117)	1:10:A:GLN:H	1:10:A:GLN:HG2	7	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB2	7	0.14	0.02	0.13
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	7	0.14	0.02	0.13
(1,187)	1:14:A:GLN:H	1:14:A:GLN:HG2	6	0.74	0.09	0.76
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB1	6	0.63	0.32	0.76
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB2	6	0.63	0.32	0.76
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB3	6	0.63	0.32	0.76
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB1	6	0.63	0.32	0.76
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB2	6	0.63	0.32	0.76
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB3	6	0.63	0.32	0.76
(1,441)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	6	0.56	0.16	0.57
(1,441)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	6	0.56	0.16	0.57
(1,441)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	6	0.56	0.16	0.57
(1,409)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	6	0.49	0.26	0.57
(1,282)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	6	0.46	0.12	0.48
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	6	0.46	0.21	0.36
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	6	0.46	0.21	0.36
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	6	0.46	0.21	0.36
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	6	0.46	0.21	0.36
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	6	0.46	0.21	0.36
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	6	0.46	0.21	0.36
(2,427)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	6	0.42	0.29	0.33
(3,393)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	6	0.42	0.29	0.33
(1,249)	1:25:A:SER:H	1:25:A:SER:HB2	6	0.37	0.13	0.4
(1,249)	1:25:A:SER:H	1:25:A:SER:HB3	6	0.37	0.13	0.4
(1,289)	1:15:A:GLY:H	1:16:A:GLY:H	6	0.32	0.18	0.24
(2,281)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	6	0.3	0.22	0.17
(3,264)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	6	0.3	0.22	0.17
(1,52)	1:6:A:ARG:HA	1:6:A:ARG:HG2	6	0.3	0.19	0.22
(1,399)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	6	0.28	0.15	0.24
(1,399)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	6	0.28	0.15	0.24
(1,399)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	6	0.28	0.15	0.24
(1,399)	1:5:A:VAL:HG21	1:8:A:TYR:HB3	6	0.28	0.15	0.24
(1,399)	1:5:A:VAL:HG22	1:8:A:TYR:HB3	6	0.28	0.15	0.24
(1,399)	1:5:A:VAL:HG23	1:8:A:TYR:HB3	6	0.28	0.15	0.24
(2,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	6	0.23	0.18	0.15
(3,423)	1:7:A:LEU:HA	1:10:A:GLN:HB2	6	0.23	0.18	0.15
(2,215)	1:22:A:PRO:HA	1:22:A:PRO:HD3	6	0.21	0.03	0.2
(4,17)	1:22:A:PRO:HA	1:22:A:PRO:HD3	6	0.21	0.03	0.2
(1,361)	1:14:A:GLN:HE22	1:21:A:ARG:HG3	6	0.2	0.11	0.16
(2,440)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	6	0.15	0.02	0.16
(2,440)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	6	0.15	0.02	0.16
(2,440)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	6	0.15	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,406)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	6	0.15	0.02	0.16
(3,406)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	6	0.15	0.02	0.16
(3,406)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	6	0.15	0.02	0.16
(1,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	6	0.15	0.01	0.15
(2,265)	1:24:A:PRO:HA	1:24:A:PRO:HD3	6	0.13	0.02	0.13
(3,248)	1:24:A:PRO:HA	1:24:A:PRO:HD3	6	0.13	0.02	0.13
(2,33)	1:4:A:ALA:HB1	1:5:A:VAL:H	6	0.12	0.01	0.12
(2,33)	1:4:A:ALA:HB2	1:5:A:VAL:H	6	0.12	0.01	0.12
(2,33)	1:4:A:ALA:HB3	1:5:A:VAL:H	6	0.12	0.01	0.12
(3,32)	1:4:A:ALA:HB1	1:5:A:VAL:H	6	0.12	0.01	0.12
(3,32)	1:4:A:ALA:HB2	1:5:A:VAL:H	6	0.12	0.01	0.12
(3,32)	1:4:A:ALA:HB3	1:5:A:VAL:H	6	0.12	0.01	0.12
(2,208)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	6	0.11	0.01	0.11
(3,193)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	6	0.11	0.01	0.11
(1,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	5	0.97	0.18	1.07
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	5	0.49	0.1	0.47
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	5	0.49	0.1	0.47
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	5	0.49	0.1	0.47
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	5	0.49	0.1	0.47
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	5	0.49	0.1	0.47
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	5	0.49	0.1	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	5	0.49	0.1	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	5	0.49	0.1	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	5	0.49	0.1	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	5	0.49	0.1	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	5	0.49	0.1	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	5	0.49	0.1	0.47
(1,359)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	0.47	0.1	0.53
(1,359)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	0.47	0.1	0.53
(1,359)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	5	0.47	0.1	0.53
(1,354)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	5	0.33	0.2	0.21
(1,25)	1:3:A:GLU:HG2	1:4:A:ALA:HA	5	0.32	0.12	0.26
(1,25)	1:3:A:GLU:HG3	1:4:A:ALA:HA	5	0.32	0.12	0.26
(1,26)	1:3:A:GLU:HG2	1:4:A:ALA:H	5	0.29	0.14	0.28
(1,26)	1:3:A:GLU:HG3	1:4:A:ALA:H	5	0.29	0.14	0.28
(1,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	5	0.29	0.02	0.29
(1,225)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.25	0.06	0.28
(1,252)	1:23:A:PRO:HA	1:24:A:PRO:HD3	5	0.24	0.11	0.21
(1,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	5	0.24	0.06	0.28
(1,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	5	0.24	0.06	0.28
(1,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	5	0.24	0.06	0.28
(1,198)	1:19:A:SER:H	1:19:A:SER:HB3	5	0.24	0.09	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	5	0.24	0.04	0.24
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	5	0.24	0.04	0.24
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	5	0.24	0.04	0.24
(2,49)	1:6:A:ARG:HA	1:6:A:ARG:HD3	5	0.2	0.07	0.18
(3,46)	1:6:A:ARG:HA	1:6:A:ARG:HD3	5	0.2	0.07	0.18
(2,387)	1:5:A:VAL:HA	1:8:A:TYR:HB2	5	0.18	0.05	0.19
(3,361)	1:5:A:VAL:HA	1:8:A:TYR:HB2	5	0.18	0.05	0.19
(1,221)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	5	0.18	0.04	0.2
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	5	0.17	0.02	0.18
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	5	0.17	0.02	0.18
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	5	0.17	0.01	0.18
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	5	0.17	0.01	0.18
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	5	0.17	0.01	0.18
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	5	0.17	0.01	0.18
(1,275)	1:21:A:ARG:HA	1:22:A:PRO:HD3	5	0.16	0.03	0.17
(1,380)	1:8:A:TYR:HA	1:24:A:PRO:HG3	5	0.16	0.04	0.16
(1,146)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	5	0.15	0.03	0.15
(1,94)	1:7:A:LEU:H	1:8:A:TYR:H	5	0.14	0.03	0.13
(2,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	5	0.14	0.02	0.14
(2,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	5	0.14	0.02	0.14
(2,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	5	0.14	0.02	0.14
(4,25)	1:7:A:LEU:HD11	1:8:A:TYR:H	5	0.14	0.02	0.14
(4,25)	1:7:A:LEU:HD12	1:8:A:TYR:H	5	0.14	0.02	0.14
(4,25)	1:7:A:LEU:HD13	1:8:A:TYR:H	5	0.14	0.02	0.14
(2,348)	1:22:A:PRO:HG2	1:25:A:SER:H	5	0.12	0.01	0.12
(2,348)	1:22:A:PRO:HG3	1:25:A:SER:H	5	0.12	0.01	0.12
(3,326)	1:22:A:PRO:HG2	1:25:A:SER:H	5	0.12	0.01	0.12
(3,326)	1:22:A:PRO:HG3	1:25:A:SER:H	5	0.12	0.01	0.12
(1,57)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	5	0.12	0.0	0.12
(1,155)	1:12:A:LEU:HA	1:16:A:GLY:H	4	0.43	0.13	0.44
(1,72)	1:6:A:ARG:HD3	1:7:A:LEU:H	4	0.42	0.26	0.4
(1,188)	1:14:A:GLN:H	1:14:A:GLN:HG3	4	0.37	0.29	0.24
(1,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	4	0.32	0.24	0.22
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	4	0.22	0.03	0.23
(3,300)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	4	0.22	0.03	0.23
(1,414)	1:12:A:LEU:HA	1:17:A:PRO:HD2	4	0.17	0.04	0.18
(2,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	4	0.15	0.01	0.15
(2,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	4	0.15	0.01	0.15
(2,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	4	0.15	0.01	0.15
(3,403)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	4	0.15	0.01	0.15
(3,403)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	4	0.15	0.01	0.15
(3,403)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	4	0.15	0.01	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,421)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	4	0.14	0.03	0.13
(1,421)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	4	0.14	0.03	0.13
(2,450)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	4	0.14	0.02	0.15
(2,450)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	4	0.14	0.02	0.15
(3,413)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	4	0.14	0.02	0.15
(3,413)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	4	0.14	0.02	0.15
(2,369)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(2,369)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(2,369)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(2,369)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(2,369)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(2,369)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(2,369)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(2,369)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(2,369)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(2,369)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(2,369)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(2,369)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	4	0.14	0.04	0.12
(3,345)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	4	0.14	0.04	0.12
(1,292)	1:11:A:TRP:HA	1:11:A:TRP:HD1	4	0.14	0.02	0.14
(2,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	4	0.13	0.02	0.14
(3,328)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	4	0.13	0.02	0.14
(2,40)	1:3:A:GLU:H	1:5:A:VAL:HB	4	0.11	0.0	0.11
(3,38)	1:3:A:GLU:H	1:5:A:VAL:HB	4	0.11	0.0	0.11
(1,60)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	3	0.9	0.03	0.89
(1,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	3	0.81	0.06	0.8
(1,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	3	0.8	0.03	0.8
(1,343)	1:10:A:GLN:HE21	1:14:A:GLN:HG3	3	0.7	0.13	0.7
(1,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	3	0.67	0.07	0.68
(1,186)	1:14:A:GLN:H	1:14:A:GLN:HB3	3	0.67	0.07	0.68
(1,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	3	0.57	0.14	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,59)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	3	0.53	0.05	0.53
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD11	3	0.51	0.04	0.51
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD12	3	0.51	0.04	0.51
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD13	3	0.51	0.04	0.51
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD11	3	0.51	0.04	0.51
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD12	3	0.51	0.04	0.51
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD13	3	0.51	0.04	0.51
(1,67)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	3	0.47	0.0	0.47
(1,370)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	3	0.44	0.13	0.48
(1,370)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	3	0.44	0.13	0.48
(1,370)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	3	0.44	0.13	0.48
(1,370)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	3	0.44	0.13	0.48
(1,370)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	3	0.44	0.13	0.48
(1,370)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	3	0.44	0.13	0.48
(1,370)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	3	0.44	0.13	0.48
(1,370)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	3	0.44	0.13	0.48
(1,370)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	3	0.44	0.13	0.48
(1,370)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	3	0.44	0.13	0.48
(1,370)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	3	0.44	0.13	0.48
(1,370)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	3	0.44	0.13	0.48
(1,329)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	3	0.41	0.22	0.34
(1,329)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	3	0.41	0.22	0.34
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB1	3	0.4	0.2	0.49
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB2	3	0.4	0.2	0.49
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB3	3	0.4	0.2	0.49
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB1	3	0.4	0.2	0.49
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB2	3	0.4	0.2	0.49
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB3	3	0.4	0.2	0.49
(2,434)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	3	0.36	0.03	0.37
(2,434)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	3	0.36	0.03	0.37
(2,434)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	3	0.36	0.03	0.37
(3,400)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	3	0.36	0.03	0.37
(3,400)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	3	0.36	0.03	0.37
(3,400)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	3	0.36	0.03	0.37
(1,313)	1:11:A:TRP:HE3	1:12:A:LEU:H	3	0.3	0.09	0.36
(2,68)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.25	0.0	0.25
(3,65)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.25	0.0	0.25
(1,51)	1:6:A:ARG:HA	1:6:A:ARG:HB3	3	0.25	0.01	0.24
(1,271)	1:20:A:GLY:H	1:20:A:GLY:HA2	3	0.23	0.03	0.22
(1,133)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	3	0.22	0.03	0.24
(2,353)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	3	0.22	0.08	0.2
(3,331)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	3	0.22	0.08	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	3	0.21	0.01	0.21
(1,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	3	0.21	0.01	0.21
(1,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	3	0.21	0.01	0.21
(1,377)	1:8:A:TYR:HA	1:11:A:TRP:HB3	3	0.16	0.03	0.18
(2,464)	1:3:A:GLU:HA	1:6:A:ARG:HB2	3	0.16	0.04	0.13
(3,424)	1:3:A:GLU:HA	1:6:A:ARG:HB2	3	0.16	0.04	0.13
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB1	3	0.15	0.05	0.13
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB2	3	0.15	0.05	0.13
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB3	3	0.15	0.05	0.13
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	3	0.14	0.01	0.15
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD21	3	0.13	0.01	0.13
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD22	3	0.13	0.01	0.13
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD23	3	0.13	0.01	0.13
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD21	3	0.13	0.01	0.13
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD22	3	0.13	0.01	0.13
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD23	3	0.13	0.01	0.13
(2,436)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	3	0.13	0.01	0.13
(2,436)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	3	0.13	0.01	0.13
(2,436)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	3	0.13	0.01	0.13
(3,402)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	3	0.13	0.01	0.13
(3,402)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	3	0.13	0.01	0.13
(3,402)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	3	0.13	0.01	0.13
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD21	3	0.12	0.02	0.11
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD22	3	0.12	0.02	0.11
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD23	3	0.12	0.02	0.11
(1,407)	1:12:A:LEU:HD21	1:17:A:PRO:HD2	3	0.12	0.01	0.11
(1,407)	1:12:A:LEU:HD22	1:17:A:PRO:HD2	3	0.12	0.01	0.11
(1,407)	1:12:A:LEU:HD23	1:17:A:PRO:HD2	3	0.12	0.01	0.11
(1,211)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	3	0.11	0.01	0.11
(1,172)	1:13:A:LYS:HA	1:13:A:LYS:HD2	2	1.49	0.05	1.49
(1,172)	1:13:A:LYS:HA	1:13:A:LYS:HD3	2	1.49	0.05	1.49
(1,127)	1:10:A:GLN:HA	1:10:A:GLN:HG2	2	1.18	0.01	1.18
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	2	1.07	0.26	1.07
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG3	2	1.07	0.26	1.07
(1,131)	1:10:A:GLN:HB2	1:10:A:GLN:HE21	2	0.82	0.02	0.82
(1,131)	1:10:A:GLN:HB3	1:10:A:GLN:HE21	2	0.82	0.02	0.82
(1,478)	1:1:A:GLU:HA	1:1:A:GLU:HG2	2	0.56	0.01	0.56
(1,478)	1:1:A:GLU:HA	1:1:A:GLU:HG3	2	0.56	0.01	0.56
(2,188)	1:14:A:GLN:H	1:14:A:GLN:HG3	2	0.5	0.01	0.5
(3,175)	1:14:A:GLN:H	1:14:A:GLN:HG3	2	0.5	0.01	0.5
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	2	0.39	0.2	0.39
(1,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	2	0.35	0.11	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB3	2	0.35	0.11	0.35
(1,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	2	0.35	0.11	0.35
(1,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB3	2	0.35	0.11	0.35
(1,435)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	2	0.32	0.03	0.32
(1,435)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	2	0.32	0.03	0.32
(1,435)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	2	0.32	0.03	0.32
(1,279)	1:21:A:ARG:HA	1:21:A:ARG:HG2	2	0.3	0.05	0.3
(1,473)	1:5:A:VAL:HA	1:8:A:TYR:HD1	2	0.27	0.07	0.27
(1,473)	1:5:A:VAL:HA	1:8:A:TYR:HD2	2	0.27	0.07	0.27
(1,472)	1:13:A:LYS:H	1:14:A:GLN:HA	2	0.24	0.01	0.24
(1,346)	1:14:A:GLN:HE21	1:14:A:GLN:HG2	2	0.22	0.02	0.22
(2,130)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.2	0.01	0.2
(3,118)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.2	0.01	0.2
(1,447)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	2	0.2	0.02	0.2
(1,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	2	0.2	0.02	0.2
(2,197)	1:19:A:SER:HA	1:19:A:SER:HB2	2	0.2	0.01	0.2
(3,183)	1:19:A:SER:HA	1:19:A:SER:HB2	2	0.2	0.01	0.2
(2,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	2	0.16	0.02	0.16
(2,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	2	0.16	0.02	0.16
(2,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	2	0.16	0.02	0.16
(2,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	2	0.16	0.02	0.16
(2,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	2	0.16	0.02	0.16
(2,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	2	0.16	0.02	0.16
(3,408)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	2	0.16	0.02	0.16
(3,408)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	2	0.16	0.02	0.16
(3,408)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	2	0.16	0.02	0.16

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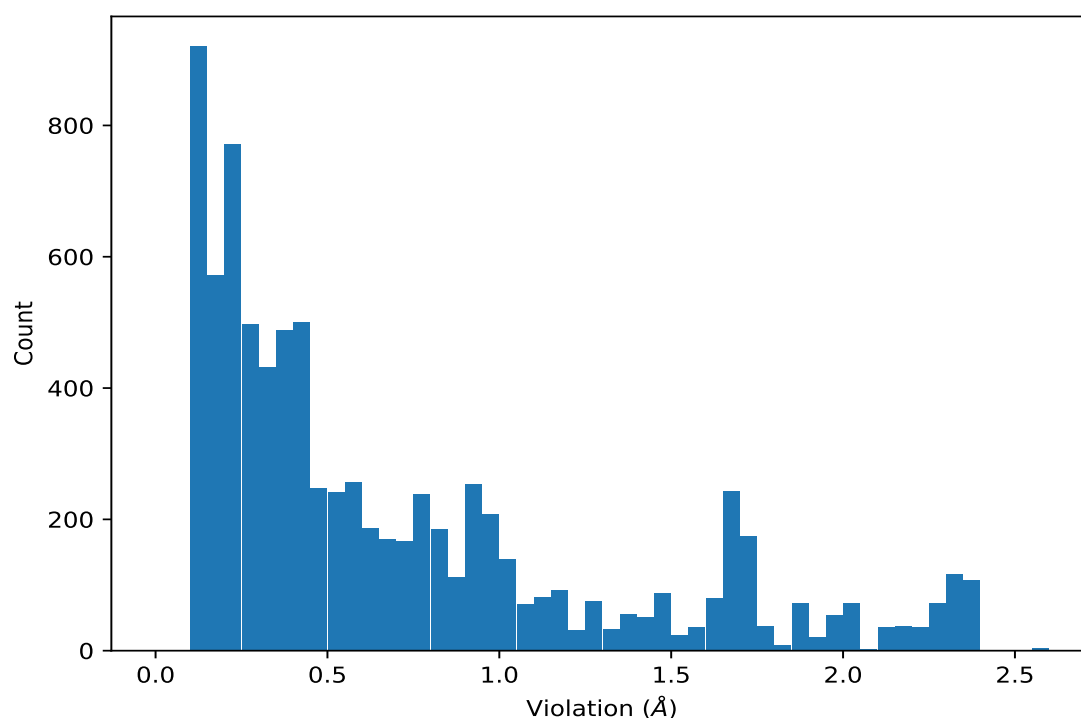
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,408)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	2	0.16	0.02	0.16
(3,408)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	2	0.16	0.02	0.16
(3,408)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	2	0.16	0.02	0.16
(1,353)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	2	0.16	0.04	0.16
(2,334)	1:12:A:LEU:HG	1:13:A:LYS:H	2	0.15	0.01	0.15
(3,313)	1:12:A:LEU:HG	1:13:A:LYS:H	2	0.15	0.01	0.15
(1,323)	1:14:A:GLN:HA	1:15:A:GLY:H	2	0.15	0.04	0.15
(2,418)	1:12:A:LEU:HG	1:13:A:LYS:HE2	2	0.12	0.02	0.12
(2,418)	1:12:A:LEU:HG	1:13:A:LYS:HE3	2	0.12	0.02	0.12
(3,386)	1:12:A:LEU:HG	1:13:A:LYS:HE2	2	0.12	0.02	0.12
(3,386)	1:12:A:LEU:HG	1:13:A:LYS:HE3	2	0.12	0.02	0.12
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HG	2	0.12	0.01	0.12
(3,83)	1:7:A:LEU:H	1:7:A:LEU:HG	2	0.12	0.01	0.12
(2,43)	1:6:A:ARG:HA	1:7:A:LEU:H	2	0.11	0.0	0.11
(2,122)	1:8:A:TYR:HA	1:10:A:GLN:H	2	0.11	0.01	0.11
(2,351)	1:13:A:LYS:HB2	1:14:A:GLN:H	2	0.11	0.01	0.11
(3,41)	1:6:A:ARG:HA	1:7:A:LEU:H	2	0.11	0.0	0.11
(3,110)	1:8:A:TYR:HA	1:10:A:GLN:H	2	0.11	0.01	0.11
(3,329)	1:13:A:LYS:HB2	1:14:A:GLN:H	2	0.11	0.01	0.11
(1,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.11	0.0	0.11
(1,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.11	0.0	0.11
(1,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.11	0.0	0.11
(1,98)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,33)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	10	2.57
(4,33)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	10	2.57
(2,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	10	2.57
(2,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	10	2.57
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	3	2.37
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	3	2.37
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	3	2.37
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	3	2.37
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	3	2.37
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	3	2.37
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	3	2.37
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	3	2.37
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	3	2.37
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	3	2.37
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	3	2.37
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	3	2.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	3	2.37
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	3	2.37
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	3	2.37
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	3	2.37
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	3	2.37
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	3	2.37
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	3	2.37
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	3	2.37
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	3	2.37
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	3	2.37
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	3	2.37
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	3	2.37
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	3	2.37
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	3	2.37
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	3	2.37
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	3	2.37
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	3	2.37
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	3	2.37
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	3	2.37
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	3	2.37
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	3	2.37
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	3	2.37
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	3	2.37
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	3	2.37
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	10	2.36
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	10	2.36
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	10	2.36
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	10	2.36
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	10	2.36
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	10	2.36
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	10	2.36
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	10	2.36
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	10	2.36
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	10	2.36
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	10	2.36
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	10	2.36
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	10	2.36
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	10	2.36
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	10	2.36
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	10	2.36
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	10	2.36
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	10	2.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	10	2.36
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	10	2.36
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	10	2.36
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	10	2.36
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	10	2.36
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	10	2.36
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	10	2.36
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	10	2.36
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	10	2.36
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	10	2.36
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	10	2.36
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	10	2.36
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	10	2.36
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	10	2.36
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	10	2.36
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	10	2.36
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	10	2.36
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	10	2.36
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	6	2.35
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	6	2.35
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	6	2.35
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	6	2.35
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	6	2.35
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	6	2.35
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	6	2.35
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	6	2.35
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	6	2.35
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	6	2.35
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	6	2.35
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	6	2.35
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	6	2.35
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	6	2.35
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	6	2.35
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	6	2.35
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	6	2.35
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	6	2.35
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	6	2.35
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	6	2.35
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	6	2.35
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	6	2.35
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	6	2.35
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	6	2.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	6	2.35
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	6	2.35
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	6	2.35
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	6	2.35
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	6	2.35
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	6	2.35
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	6	2.35
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	6	2.35
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	6	2.35
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	6	2.35
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	6	2.35
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	6	2.35
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	5	2.34
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	5	2.34
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	5	2.34
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	5	2.34
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	5	2.34
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	5	2.34
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	5	2.34
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	5	2.34
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	5	2.34
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	5	2.34
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	5	2.34
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	5	2.34
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	5	2.34
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	5	2.34
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	5	2.34
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	5	2.34
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	5	2.34
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	5	2.34
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	9	2.34
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	9	2.34
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	9	2.34
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	9	2.34
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	9	2.34
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	9	2.34
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	9	2.34
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	9	2.34
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	9	2.34
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	9	2.34
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	9	2.34
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	9	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	9	2.34
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	9	2.34
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	9	2.34
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	9	2.34
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	9	2.34
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	9	2.34
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	5	2.34
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	5	2.34
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	5	2.34
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	5	2.34
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	5	2.34
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	5	2.34
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	5	2.34
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	5	2.34
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	5	2.34
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	5	2.34
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	5	2.34
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	5	2.34
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	5	2.34
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	5	2.34
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	5	2.34
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	5	2.34
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	5	2.34
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	5	2.34
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	9	2.34
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	9	2.34
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	9	2.34
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	9	2.34
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	9	2.34
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	9	2.34
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	9	2.34
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	9	2.34
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	9	2.34
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	9	2.34
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	9	2.34
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	9	2.34
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	9	2.34
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	9	2.34
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	9	2.34
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	9	2.34
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	9	2.34
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	9	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,404)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	2.32
(3,404)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	2.32
(3,404)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	2.32
(2,438)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	2.32
(2,438)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	2.32
(2,438)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	2.32
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	2	2.31
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	2	2.31
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	2	2.31
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	2	2.31
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	2	2.31
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	2	2.31
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	2	2.31
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	2	2.31
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	2	2.31
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	2	2.31
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	2	2.31
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	2	2.31
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	2	2.31
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	2	2.31
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	2	2.31
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	2	2.31
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	2	2.31
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	2	2.31
(4,32)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	6	2.31
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	2	2.31
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	2	2.31
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	2	2.31
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	2	2.31
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	2	2.31
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	2	2.31
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	2	2.31
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	2	2.31
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	2	2.31
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	2	2.31
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	2	2.31
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	2	2.31
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	2	2.31
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	2	2.31
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	2	2.31
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	2	2.31
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	2	2.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	2	2.31
(2,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	6	2.31
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	4	2.3
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	4	2.3
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	4	2.3
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	4	2.3
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	4	2.3
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	4	2.3
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	4	2.3
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	4	2.3
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	4	2.3
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	4	2.3
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	4	2.3
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	4	2.3
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	4	2.3
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	4	2.3
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	4	2.3
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	4	2.3
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	4	2.3
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	4	2.3
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	4	2.3
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	4	2.3
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	4	2.3
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	4	2.3
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	4	2.3
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	4	2.3
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	4	2.3
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	4	2.3
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	4	2.3
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	4	2.3
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	4	2.3
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	4	2.3
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	4	2.3
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	4	2.3
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	4	2.3
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	4	2.3
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	4	2.3
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	4	2.3
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	1	2.28
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	1	2.28
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	1	2.28
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	1	2.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	1	2.28
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	1	2.28
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	1	2.28
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	1	2.28
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	1	2.28
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	1	2.28
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	1	2.28
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	1	2.28
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	1	2.28
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	1	2.28
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	1	2.28
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	1	2.28
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	1	2.28
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	1	2.28
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	1	2.28
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	1	2.28
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	1	2.28
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	1	2.28
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	1	2.28
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	1	2.28
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	1	2.28
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	1	2.28
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	1	2.28
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	1	2.28
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	1	2.28
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	1	2.28
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	1	2.28
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	1	2.28
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	1	2.28
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	1	2.28
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	1	2.28
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	1	2.28
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	7	2.24
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	7	2.24
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	7	2.24
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	7	2.24
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	7	2.24
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	7	2.24
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	7	2.24
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	7	2.24
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	7	2.24
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	7	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	7	2.24
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	7	2.24
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	7	2.24
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	7	2.24
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	7	2.24
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	7	2.24
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	7	2.24
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	7	2.24
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	7	2.24
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	7	2.24
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	7	2.24
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	7	2.24
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	7	2.24
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	7	2.24
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	7	2.24
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	7	2.24
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	7	2.24
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	7	2.24
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	7	2.24
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	7	2.24
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	7	2.24
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	7	2.24
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	7	2.24
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	7	2.24
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	7	2.24
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	7	2.24
(4,23)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	3	2.19
(2,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	3	2.19
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	8	2.16
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	8	2.16
(4,36)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	8	2.16
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	8	2.16
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	8	2.16
(4,36)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	8	2.16
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	8	2.16
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	8	2.16
(4,36)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	8	2.16
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	8	2.16
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	8	2.16
(4,36)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	8	2.16
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	8	2.16
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	8	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,36)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	8	2.16
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	8	2.16
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	8	2.16
(4,36)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	8	2.16
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	8	2.16
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	8	2.16
(2,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	8	2.16
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	8	2.16
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	8	2.16
(2,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	8	2.16
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	8	2.16
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	8	2.16
(2,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	8	2.16
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	8	2.16
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	8	2.16
(2,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	8	2.16
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	8	2.16
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	8	2.16
(2,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	8	2.16
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	8	2.16
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	8	2.16
(2,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	8	2.16
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	8	2.14
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	8	2.14
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	8	2.14
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	8	2.14
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	8	2.14
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	8	2.14
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	8	2.14
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	8	2.14
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	8	2.14
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	8	2.14
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	8	2.14
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	8	2.14
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	8	2.14
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	8	2.14
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	8	2.14
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	8	2.14
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	8	2.14
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	8	2.14
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	8	2.14
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	8	2.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	8	2.14
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	8	2.14
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	8	2.14
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	8	2.14
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	8	2.14
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	8	2.14
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	8	2.14
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	8	2.14
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	8	2.14
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	8	2.14
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	8	2.14
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	8	2.14
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	8	2.14
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	8	2.14
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	8	2.14
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	8	2.14
(4,23)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	6	2.07
(2,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	6	2.07
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	6	2.02
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	6	2.02
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	6	2.02
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	6	2.02
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	6	2.02
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	6	2.02
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	6	2.02
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	6	2.02
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	6	2.02
(3,412)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	1	2.02
(3,412)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	1	2.02
(3,412)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	1	2.02
(3,412)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	1	2.02
(3,412)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	1	2.02
(3,412)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	1	2.02
(3,412)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	1	2.02
(3,412)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	1	2.02
(3,412)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	1	2.02
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	6	2.02
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	6	2.02
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	6	2.02
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	6	2.02
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	6	2.02
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	6	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	6	2.02
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	6	2.02
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	6	2.02
(2,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	1	2.02
(2,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	1	2.02
(2,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	1	2.02
(2,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	1	2.02
(2,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	1	2.02
(2,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	1	2.02
(2,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	1	2.02
(2,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	1	2.02
(2,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	1	2.02
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	6	2.0
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	6	2.0
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	6	2.0
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	6	2.0
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	6	2.0
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	6	2.0
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	6	2.0
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	6	2.0
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	6	2.0
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	6	2.0
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	6	2.0
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	6	2.0
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	6	2.0
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	6	2.0
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	6	2.0
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	6	2.0
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	6	2.0
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	6	2.0
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	6	2.0
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	6	2.0
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	6	2.0
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	6	2.0
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	6	2.0
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	6	2.0
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	6	2.0
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	6	2.0
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	6	2.0
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	6	2.0
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	6	2.0
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	6	2.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	6	2.0
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	6	2.0
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	6	2.0
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	6	2.0
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	6	2.0
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	6	2.0
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	9	1.99
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	9	1.99
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	9	1.99
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	9	1.99
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	9	1.99
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	9	1.99
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	9	1.99
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	9	1.99
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	9	1.99
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	9	1.99
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	9	1.99
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	9	1.99
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	9	1.99
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	9	1.99
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	9	1.99
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	9	1.99
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	9	1.99
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	9	1.99
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	9	1.99
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	9	1.99
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	9	1.99
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	9	1.99
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	9	1.99
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	9	1.99
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	9	1.99
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	9	1.99
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	9	1.99
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	9	1.99
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	9	1.99
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	9	1.99
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	9	1.99
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	9	1.99
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	9	1.99
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	9	1.99
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	9	1.99
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	9	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	1	1.97
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	1	1.97
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	1	1.97
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	1	1.97
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	1	1.97
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	1	1.97
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	1	1.97
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	1	1.97
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	1	1.97
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	1	1.97
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	1	1.97
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	1	1.97
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	1	1.97
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	1	1.97
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	1	1.97
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	1	1.97
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	1	1.97
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	1	1.97
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	3	1.92
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	3	1.92
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	3	1.92
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	3	1.92
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	3	1.92
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	3	1.92
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	3	1.92
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	3	1.92
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	3	1.92
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	3	1.92
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	3	1.92
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	3	1.92
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	3	1.92
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	3	1.92
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	3	1.92
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	3	1.92
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	3	1.92
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	3	1.92
(4,32)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	2	1.91
(2,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	2	1.91
(4,23)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	9	1.89
(4,23)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	10	1.89
(2,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	9	1.89
(2,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	10	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	10	1.89
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	10	1.89
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	10	1.89
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	10	1.89
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	3	1.88
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	3	1.88
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	3	1.88
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	3	1.88
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	3	1.88
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	3	1.88
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	3	1.88
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	3	1.88
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	3	1.88
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	3	1.88
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	3	1.88
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	3	1.88
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	3	1.88
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	3	1.88
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	3	1.88
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	3	1.88
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	3	1.88
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	3	1.88
(4,30)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	1	1.88
(3,360)	1:15:A:GLY:HA3	1:18:A:SER:HB3	5	1.88
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	3	1.88
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	3	1.88
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	3	1.88
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	3	1.88
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	3	1.88
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	3	1.88
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	3	1.88
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	3	1.88
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	3	1.88
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	3	1.88
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	3	1.88
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	3	1.88
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	3	1.88
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	3	1.88
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	3	1.88
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	3	1.88
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	3	1.88
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	3	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	1	1.88
(2,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	5	1.88
(4,23)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	7	1.87
(2,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	7	1.87
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	9	1.86
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	9	1.86
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	9	1.86
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	9	1.86
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	9	1.86
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	9	1.86
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	9	1.86
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	9	1.86
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	9	1.86
(4,32)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	1	1.86
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	9	1.86
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	9	1.86
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	9	1.86
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	9	1.86
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	9	1.86
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	9	1.86
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	9	1.86
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	9	1.86
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	9	1.86
(2,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	1	1.86
(4,30)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	2	1.85
(2,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	2	1.85
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG11	1	1.84
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG12	1	1.84
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG13	1	1.84
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG11	1	1.84
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG12	1	1.84
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG13	1	1.84
(3,360)	1:15:A:GLY:HA3	1:18:A:SER:HB3	7	1.83
(2,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	7	1.83
(3,360)	1:15:A:GLY:HA3	1:18:A:SER:HB3	3	1.79
(2,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	3	1.79
(4,33)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	4	1.78
(4,33)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	4	1.78
(4,32)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	9	1.78
(2,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	4	1.78
(2,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	4	1.78
(2,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	9	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	10	1.77
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	10	1.77
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	10	1.77
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	10	1.77
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	10	1.77
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	10	1.77
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	10	1.77
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	10	1.77
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	10	1.77
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	10	1.77
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	10	1.77
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	10	1.77
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	10	1.77
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	10	1.77
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	10	1.77
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	10	1.77
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	10	1.77
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	10	1.77
(4,33)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	3	1.76
(4,33)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	3	1.76
(4,32)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	4	1.76
(2,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	3	1.76
(2,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	3	1.76
(2,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	4	1.76
(1,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	10	1.76
(1,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	10	1.76
(1,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	10	1.76
(4,30)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	9	1.75
(2,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	9	1.75
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	2	1.74
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	2	1.74
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	2	1.74
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	2	1.74
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	2	1.74
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	2	1.74
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	2	1.74
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	2	1.74
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	2	1.74
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	5	1.74
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	5	1.74
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	5	1.74
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	5	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	5	1.74
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	5	1.74
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	5	1.74
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	5	1.74
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	5	1.74
(4,30)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	5	1.74
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	2	1.74
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	2	1.74
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	2	1.74
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	2	1.74
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	2	1.74
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	2	1.74
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	2	1.74
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	2	1.74
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	2	1.74
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	5	1.74
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	5	1.74
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	5	1.74
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	5	1.74
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	5	1.74
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	5	1.74
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	5	1.74
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	5	1.74
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	5	1.74
(2,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	5	1.74
(1,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	7	1.74
(1,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	7	1.74
(1,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	7	1.74
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	3	1.74
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	3	1.74
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	3	1.74
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	3	1.74
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	7	1.73
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	7	1.73
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	7	1.73
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	7	1.73
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	7	1.73
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	7	1.73
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	7	1.73
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	7	1.73
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	7	1.73
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	7	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	7	1.73
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	7	1.73
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	7	1.73
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	7	1.73
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	7	1.73
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	7	1.73
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	7	1.73
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	7	1.73
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	1	1.73
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	1	1.73
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	1	1.73
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	1	1.73
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	1	1.73
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	1	1.73
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	1	1.73
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	1	1.73
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	1	1.73
(4,30)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	4	1.73
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	7	1.73
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	7	1.73
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	7	1.73
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	7	1.73
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	7	1.73
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	7	1.73
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	7	1.73
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	7	1.73
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	7	1.73
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	7	1.73
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	7	1.73
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	7	1.73
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	7	1.73
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	7	1.73
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	7	1.73
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	7	1.73
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	7	1.73
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	7	1.73
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	1	1.73
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	1	1.73
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	1	1.73
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	1	1.73
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	1	1.73
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	1	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	1	1.73
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	1	1.73
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	1	1.73
(2,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	4	1.73
(1,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	6	1.73
(1,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	6	1.73
(1,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	6	1.73
(4,33)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	6	1.72
(4,33)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	6	1.72
(4,33)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	9	1.72
(4,33)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	9	1.72
(2,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	6	1.72
(2,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	6	1.72
(2,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	9	1.72
(2,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	9	1.72
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	5	1.72
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	5	1.72
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	5	1.72
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	5	1.72
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	4	1.71
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	4	1.71
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	4	1.71
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	4	1.71
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	4	1.71
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	4	1.71
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	4	1.71
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	4	1.71
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	4	1.71
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	4	1.71
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	4	1.71
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	4	1.71
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	4	1.71
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	4	1.71
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	4	1.71
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	4	1.71
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	4	1.71
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	4	1.71
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	4	1.71
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	4	1.71
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	4	1.71
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	4	1.71
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	4	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	4	1.71
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	4	1.71
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	4	1.71
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	4	1.71
(4,33)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	2	1.71
(4,33)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	2	1.71
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	4	1.71
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	4	1.71
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	4	1.71
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	4	1.71
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	4	1.71
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	4	1.71
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	4	1.71
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	4	1.71
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	4	1.71
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	4	1.71
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	4	1.71
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	4	1.71
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	4	1.71
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	4	1.71
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	4	1.71
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	4	1.71
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	4	1.71
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	4	1.71
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	4	1.71
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	4	1.71
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	4	1.71
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	4	1.71
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	4	1.71
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	4	1.71
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	4	1.71
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	4	1.71
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	4	1.71
(2,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	2	1.71
(2,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	2	1.71
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	2	1.7
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	2	1.7
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	2	1.7
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	2	1.7
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	2	1.7
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	2	1.7
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	2	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	2	1.7
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	2	1.7
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	2	1.7
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	2	1.7
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	2	1.7
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	2	1.7
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	2	1.7
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	2	1.7
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	2	1.7
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	2	1.7
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	2	1.7
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	10	1.7
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	10	1.7
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	10	1.7
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	10	1.7
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	10	1.7
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	10	1.7
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	10	1.7
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	10	1.7
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	10	1.7
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	10	1.7
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	10	1.7
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	10	1.7
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	10	1.7
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	10	1.7
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	10	1.7
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	10	1.7
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	10	1.7
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	10	1.7
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	8	1.7
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	8	1.7
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	8	1.7
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	8	1.7
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	8	1.7
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	8	1.7
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	8	1.7
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	8	1.7
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	8	1.7
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	2	1.7
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	2	1.7
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	2	1.7
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	2	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	2	1.7
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	2	1.7
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	2	1.7
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	2	1.7
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	2	1.7
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	2	1.7
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	2	1.7
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	2	1.7
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	2	1.7
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	2	1.7
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	2	1.7
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	2	1.7
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	2	1.7
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	2	1.7
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	10	1.7
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	10	1.7
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	10	1.7
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	10	1.7
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	10	1.7
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	10	1.7
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	10	1.7
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	10	1.7
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	10	1.7
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	10	1.7
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	10	1.7
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	10	1.7
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	10	1.7
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	10	1.7
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	10	1.7
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	10	1.7
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	10	1.7
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	10	1.7
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	8	1.7
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	8	1.7
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	8	1.7
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	8	1.7
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	8	1.7
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	8	1.7
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	8	1.7
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	8	1.7
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	8	1.7
(1,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	3	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	3	1.7
(1,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	3	1.7
(1,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	5	1.7
(1,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	5	1.7
(1,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	5	1.7
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	5	1.69
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	5	1.69
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	5	1.69
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	5	1.69
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	5	1.69
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	5	1.69
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	5	1.69
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	5	1.69
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	5	1.69
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	5	1.69
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	5	1.69
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	5	1.69
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	5	1.69
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	5	1.69
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	5	1.69
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	5	1.69
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	5	1.69
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	5	1.69
(4,33)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	5	1.69
(4,33)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	5	1.69
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	5	1.69
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	5	1.69
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	5	1.69
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	5	1.69
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	5	1.69
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	5	1.69
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	5	1.69
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	5	1.69
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	5	1.69
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	5	1.69
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	5	1.69
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	5	1.69
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	5	1.69
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	5	1.69
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	5	1.69
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	5	1.69
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	5	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	5	1.69
(2,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	5	1.69
(2,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	5	1.69
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	3	1.69
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	3	1.69
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	3	1.69
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	3	1.69
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	3	1.69
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	3	1.69
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	3	1.69
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	3	1.69
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	3	1.69
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	3	1.69
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	3	1.69
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	3	1.69
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	3	1.69
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	3	1.69
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	3	1.69
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	3	1.69
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	3	1.69
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	3	1.69
(1,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	1	1.69
(1,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	1	1.69
(1,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	1	1.69
(1,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	8	1.69
(1,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	8	1.69
(1,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	8	1.69
(1,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	9	1.69
(1,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	9	1.69
(1,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	9	1.69
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	10	1.68
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	10	1.68
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	10	1.68
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	10	1.68
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	10	1.68
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	10	1.68
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	10	1.68
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	10	1.68
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	10	1.68
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	10	1.68
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	10	1.68
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	10	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	10	1.68
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	10	1.68
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	10	1.68
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	10	1.68
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	10	1.68
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	10	1.68
(4,39)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	1.67
(4,39)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	1.67
(4,32)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	5	1.67
(2,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	1.67
(2,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	1.67
(2,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	5	1.67
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	6	1.67
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	6	1.67
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	6	1.67
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	6	1.67
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	6	1.67
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	6	1.67
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	6	1.67
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	6	1.67
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	6	1.67
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	6	1.67
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	6	1.67
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	6	1.67
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	6	1.67
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	6	1.67
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	6	1.67
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	6	1.67
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	6	1.67
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	6	1.67
(4,23)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	5	1.66
(2,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	5	1.66
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	5	1.66
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	5	1.66
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	5	1.66
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	5	1.66
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	5	1.66
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	5	1.66
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	5	1.66
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	5	1.66
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	5	1.66
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	5	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	5	1.66
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	5	1.66
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	5	1.66
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	5	1.66
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	5	1.66
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	5	1.66
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	5	1.66
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	5	1.66
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	9	1.66
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	9	1.66
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	9	1.66
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	9	1.66
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	9	1.66
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	9	1.66
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	9	1.66
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	9	1.66
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	9	1.66
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	9	1.66
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	9	1.66
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	9	1.66
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	9	1.66
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	9	1.66
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	9	1.66
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	9	1.66
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	9	1.66
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	9	1.66
(1,392)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	9	1.65
(4,39)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	3	1.64
(4,39)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	3	1.64
(4,23)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	1	1.64
(2,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	3	1.64
(2,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	3	1.64
(2,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	1	1.64
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	2	1.63
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	2	1.63
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	2	1.63
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	2	1.63
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	2	1.63
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	2	1.63
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	2	1.63
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	2	1.63
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	2	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	2	1.63
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	2	1.63
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	2	1.63
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	2	1.63
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	2	1.63
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	2	1.63
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	2	1.63
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	2	1.63
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	2	1.63
(1,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	2	1.63
(1,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	2	1.63
(1,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	2	1.63
(3,370)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	3	1.62
(3,370)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	3	1.62
(3,370)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	3	1.62
(2,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	3	1.62
(2,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	3	1.62
(2,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	3	1.62
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	4	1.62
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	4	1.62
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	4	1.62
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	4	1.62
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	4	1.62
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	4	1.62
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	4	1.62
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	4	1.62
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	4	1.62
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	4	1.62
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	4	1.62
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	4	1.62
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	4	1.62
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	4	1.62
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	4	1.62
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	4	1.62
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	4	1.62
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	4	1.62
(1,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	4	1.62
(1,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	4	1.62
(1,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	4	1.62
(1,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	6	1.61
(3,370)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	7	1.6
(3,370)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	7	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,370)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	7	1.6
(2,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	7	1.6
(2,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	7	1.6
(2,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	7	1.6
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	1	1.6
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	1	1.6
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	1	1.6
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	1	1.6
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	1	1.6
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	1	1.6
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	1	1.6
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	1	1.6
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	1	1.6
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	1	1.6
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	1	1.6
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	1	1.6
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	1	1.6
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	1	1.6
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	1	1.6
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	1	1.6
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	1	1.6
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	1	1.6
(4,23)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	2	1.59
(3,382)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	5	1.59
(3,360)	1:15:A:GLY:HA3	1:18:A:SER:HB3	1	1.59
(2,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	5	1.59
(2,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	1	1.59
(2,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	2	1.59
(3,370)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	6	1.58
(3,370)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	6	1.58
(3,370)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	6	1.58
(2,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	6	1.58
(2,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	6	1.58
(2,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	6	1.58
(4,39)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	8	1.56
(4,39)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	8	1.56
(2,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	8	1.56
(2,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	8	1.56
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	7	1.56
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	7	1.56
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	7	1.56
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	7	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	7	1.56
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	7	1.56
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	7	1.56
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	7	1.56
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	7	1.56
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	7	1.56
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	7	1.56
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	7	1.56
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	7	1.56
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	7	1.56
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	7	1.56
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	7	1.56
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	7	1.56
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	7	1.56
(1,392)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	2	1.56
(1,392)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	10	1.55
(4,39)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	9	1.54
(4,39)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	9	1.54
(3,370)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	8	1.54
(3,370)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	8	1.54
(3,370)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	8	1.54
(2,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	9	1.54
(2,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	9	1.54
(2,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	8	1.54
(2,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	8	1.54
(2,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	8	1.54
(1,172)	1:13:A:LYS:HA	1:13:A:LYS:HD2	3	1.54
(1,172)	1:13:A:LYS:HA	1:13:A:LYS:HD3	3	1.54
(1,396)	1:12:A:LEU:HD21	1:17:A:PRO:HD3	5	1.52
(1,396)	1:12:A:LEU:HD22	1:17:A:PRO:HD3	5	1.52
(1,396)	1:12:A:LEU:HD23	1:17:A:PRO:HD3	5	1.52
(1,396)	1:12:A:LEU:HD21	1:17:A:PRO:HD3	9	1.52
(1,396)	1:12:A:LEU:HD22	1:17:A:PRO:HD3	9	1.52
(1,396)	1:12:A:LEU:HD23	1:17:A:PRO:HD3	9	1.52
(1,392)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	5	1.52
(3,382)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	7	1.5
(2,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	7	1.5
(1,392)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	1	1.5
(1,392)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	3	1.5
(1,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	3	1.5
(1,396)	1:12:A:LEU:HD21	1:17:A:PRO:HD3	4	1.49
(1,396)	1:12:A:LEU:HD22	1:17:A:PRO:HD3	4	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:12:A:LEU:HD23	1:17:A:PRO:HD3	4	1.49
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	1	1.48
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	1	1.48
(4,38)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	1	1.48
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	1	1.48
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	1	1.48
(4,38)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	1	1.48
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	1	1.48
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	1	1.48
(4,38)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	1	1.48
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	1	1.48
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	1	1.48
(4,38)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	1	1.48
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	1	1.48
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	1	1.48
(4,38)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	1	1.48
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	1	1.48
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	1	1.48
(4,38)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	1	1.48
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	7	1.48
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	7	1.48
(4,37)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	7	1.48
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	7	1.48
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	7	1.48
(4,37)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	7	1.48
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	7	1.48
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	7	1.48
(4,37)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	7	1.48
(4,30)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	7	1.48
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	1	1.48
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	1	1.48
(2,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	1	1.48
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	1	1.48
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	1	1.48
(2,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	1	1.48
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	1	1.48
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	1	1.48
(2,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	1	1.48
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	1	1.48
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	1	1.48
(2,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	1	1.48
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	1	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	1	1.48
(2,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	1	1.48
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	1	1.48
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	1	1.48
(2,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	1	1.48
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	7	1.48
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	7	1.48
(2,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	7	1.48
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	7	1.48
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	7	1.48
(2,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	7	1.48
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	7	1.48
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	7	1.48
(2,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	7	1.48
(2,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	7	1.48
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD21	8	1.48
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD22	8	1.48
(1,448)	1:5:A:VAL:HG11	1:7:A:LEU:HD23	8	1.48
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD21	8	1.48
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD22	8	1.48
(1,448)	1:5:A:VAL:HG12	1:7:A:LEU:HD23	8	1.48
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD21	8	1.48
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD22	8	1.48
(1,448)	1:5:A:VAL:HG13	1:7:A:LEU:HD23	8	1.48
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD21	8	1.48
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD22	8	1.48
(1,448)	1:5:A:VAL:HG21	1:7:A:LEU:HD23	8	1.48
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD21	8	1.48
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD22	8	1.48
(1,448)	1:5:A:VAL:HG22	1:7:A:LEU:HD23	8	1.48
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD21	8	1.48
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD22	8	1.48
(1,448)	1:5:A:VAL:HG23	1:7:A:LEU:HD23	8	1.48
(1,396)	1:12:A:LEU:HD21	1:17:A:PRO:HD3	1	1.48
(1,396)	1:12:A:LEU:HD22	1:17:A:PRO:HD3	1	1.48
(1,396)	1:12:A:LEU:HD23	1:17:A:PRO:HD3	1	1.48
(1,392)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	4	1.48
(3,281)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	6	1.47
(2,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	6	1.47
(4,39)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	6	1.46
(4,39)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	6	1.46
(2,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	6	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	6	1.46
(4,30)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	6	1.45
(3,382)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	6	1.45
(2,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	6	1.45
(2,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	6	1.45
(1,396)	1:12:A:LEU:HD21	1:17:A:PRO:HD3	2	1.45
(1,396)	1:12:A:LEU:HD22	1:17:A:PRO:HD3	2	1.45
(1,396)	1:12:A:LEU:HD23	1:17:A:PRO:HD3	2	1.45
(1,396)	1:12:A:LEU:HD21	1:17:A:PRO:HD3	10	1.45
(1,396)	1:12:A:LEU:HD22	1:17:A:PRO:HD3	10	1.45
(1,396)	1:12:A:LEU:HD23	1:17:A:PRO:HD3	10	1.45
(3,281)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	7	1.44
(2,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	7	1.44
(1,237)	1:23:A:PRO:HA	1:23:A:PRO:HG3	6	1.44
(1,172)	1:13:A:LYS:HA	1:13:A:LYS:HD2	5	1.44
(1,172)	1:13:A:LYS:HA	1:13:A:LYS:HD3	5	1.44
(1,392)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	7	1.43
(1,392)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	8	1.43
(1,367)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	8	1.43
(1,367)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	8	1.43
(1,367)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	9	1.43
(1,367)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	9	1.43
(1,237)	1:23:A:PRO:HA	1:23:A:PRO:HG3	3	1.43
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE2	6	1.43
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE3	6	1.43
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE2	4	1.42
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE3	4	1.42
(4,23)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	4	1.41
(2,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	4	1.41
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	8	1.41
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	8	1.41
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	8	1.41
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	8	1.41
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	8	1.41
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	8	1.41
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	8	1.41
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	8	1.41
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	8	1.41
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	8	1.41
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	8	1.41
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	8	1.41
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	8	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	8	1.41
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	8	1.41
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	8	1.41
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	8	1.41
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	8	1.41
(1,392)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	6	1.41
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	4	1.41
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	4	1.41
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	4	1.41
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	4	1.41
(1,237)	1:23:A:PRO:HA	1:23:A:PRO:HG3	2	1.4
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE2	2	1.4
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE3	2	1.4
(4,30)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	8	1.39
(3,394)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	10	1.39
(3,360)	1:15:A:GLY:HA3	1:18:A:SER:HB3	6	1.39
(2,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	10	1.39
(2,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	8	1.39
(2,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	6	1.39
(1,367)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	3	1.39
(1,367)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	3	1.39
(1,237)	1:23:A:PRO:HA	1:23:A:PRO:HG3	1	1.39
(1,237)	1:23:A:PRO:HA	1:23:A:PRO:HG3	5	1.39
(1,237)	1:23:A:PRO:HA	1:23:A:PRO:HG3	10	1.39
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	6	1.39
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	6	1.39
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	6	1.39
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	6	1.39
(3,281)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	5	1.38
(2,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	5	1.38
(1,237)	1:23:A:PRO:HA	1:23:A:PRO:HG3	9	1.38
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	2	1.38
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	2	1.38
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	2	1.38
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	2	1.38
(4,23)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	8	1.37
(3,37)	1:4:A:ALA:H	1:5:A:VAL:HG11	1	1.37
(3,37)	1:4:A:ALA:H	1:5:A:VAL:HG12	1	1.37
(3,37)	1:4:A:ALA:H	1:5:A:VAL:HG13	1	1.37
(2,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	8	1.37
(2,38)	1:4:A:ALA:H	1:5:A:VAL:HG11	1	1.37
(2,38)	1:4:A:ALA:H	1:5:A:VAL:HG12	1	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:4:A:ALA:H	1:5:A:VAL:HG13	1	1.37
(1,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	6	1.37
(1,237)	1:23:A:PRO:HA	1:23:A:PRO:HG3	4	1.37
(1,237)	1:23:A:PRO:HA	1:23:A:PRO:HG3	7	1.37
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	9	1.37
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	9	1.37
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	9	1.37
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	9	1.37
(3,417)	1:5:A:VAL:HG21	1:9:A:ILE:H	1	1.36
(3,417)	1:5:A:VAL:HG22	1:9:A:ILE:H	1	1.36
(3,417)	1:5:A:VAL:HG23	1:9:A:ILE:H	1	1.36
(3,281)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	1	1.36
(3,281)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	3	1.36
(3,281)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	4	1.36
(2,455)	1:5:A:VAL:HG21	1:9:A:ILE:H	1	1.36
(2,455)	1:5:A:VAL:HG22	1:9:A:ILE:H	1	1.36
(2,455)	1:5:A:VAL:HG23	1:9:A:ILE:H	1	1.36
(2,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	1	1.36
(2,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	3	1.36
(2,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	4	1.36
(1,237)	1:23:A:PRO:HA	1:23:A:PRO:HG3	8	1.36
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE2	8	1.35
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE3	8	1.35
(3,281)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	2	1.34
(3,281)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	8	1.34
(2,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	2	1.34
(2,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	8	1.34
(1,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	10	1.34
(4,32)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	8	1.33
(3,280)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	1.33
(2,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	8	1.33
(2,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	1.33
(1,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	9	1.33
(1,318)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	7	1.33
(1,255)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	6	1.33
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	10	1.33
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG3	10	1.33
(1,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	10	1.31
(1,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	10	1.31
(1,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	10	1.31
(1,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	5	1.31
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	6	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	6	1.3
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	6	1.3
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	6	1.3
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	6	1.3
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	6	1.3
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	6	1.3
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	6	1.3
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	6	1.3
(1,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	8	1.3
(1,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	8	1.3
(1,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	8	1.3
(1,367)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	6	1.3
(1,367)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	6	1.3
(3,410)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	1	1.29
(3,410)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	1	1.29
(3,410)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	1	1.29
(2,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	1	1.29
(2,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	1	1.29
(2,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	1	1.29
(1,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	3	1.29
(1,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	3	1.29
(1,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	3	1.29
(1,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	7	1.29
(1,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	7	1.29
(1,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	7	1.29
(1,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	4	1.29
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	7	1.29
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	7	1.29
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	7	1.29
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	7	1.29
(4,32)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	7	1.28
(3,280)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	1.28
(3,280)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.28
(2,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	7	1.28
(2,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	1.28
(2,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.28
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	6	1.28
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	6	1.28
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	6	1.28
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	6	1.28
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	6	1.28
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	6	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	6	1.28
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	6	1.28
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	6	1.28
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	6	1.28
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	6	1.28
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	6	1.28
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	6	1.28
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	6	1.28
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	6	1.28
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	6	1.28
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	6	1.28
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	6	1.28
(1,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	3	1.28
(1,318)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	6	1.28
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	9	1.27
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	9	1.27
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	9	1.27
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	9	1.27
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	9	1.27
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	9	1.27
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	9	1.27
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	9	1.27
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	9	1.27
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	9	1.27
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	9	1.27
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	9	1.27
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	9	1.27
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	9	1.27
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	9	1.27
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	9	1.27
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	9	1.27
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	9	1.27
(1,367)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	10	1.27
(1,367)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	10	1.27
(4,39)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	1	1.26
(4,39)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	1	1.26
(3,281)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	1.26
(2,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	1	1.26
(2,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	1	1.26
(2,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	1.26
(1,404)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	8	1.26
(1,404)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	8	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	8	1.26
(3,339)	1:14:A:GLN:HE22	1:21:A:ARG:HG2	1	1.25
(3,281)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	9	1.25
(2,362)	1:14:A:GLN:HE22	1:21:A:ARG:HG2	1	1.25
(2,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	9	1.25
(3,280)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	1.24
(2,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	1.24
(3,383)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	1.23
(3,280)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	1.23
(2,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	1.23
(2,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	1.23
(1,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	5	1.23
(1,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	5	1.23
(1,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	5	1.23
(1,367)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	7	1.23
(1,367)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	7	1.23
(1,73)	1:6:A:ARG:HD2	1:7:A:LEU:H	7	1.23
(1,58)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	3	1.23
(3,383)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	1	1.22
(2,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	1	1.22
(1,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	2	1.22
(1,404)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	7	1.22
(1,404)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	7	1.22
(1,404)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	7	1.22
(1,404)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	10	1.22
(1,404)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	10	1.22
(1,404)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	10	1.22
(4,32)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	3	1.21
(2,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	3	1.21
(1,396)	1:12:A:LEU:HD21	1:17:A:PRO:HD3	8	1.21
(1,396)	1:12:A:LEU:HD22	1:17:A:PRO:HD3	8	1.21
(1,396)	1:12:A:LEU:HD23	1:17:A:PRO:HD3	8	1.21
(1,330)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	7	1.21
(1,330)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	7	1.21
(1,318)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	3	1.21
(1,73)	1:6:A:ARG:HD2	1:7:A:LEU:H	6	1.21
(4,39)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	7	1.2
(4,39)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	7	1.2
(3,383)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	1.2
(2,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	7	1.2
(2,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	7	1.2
(2,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG11	9	1.2
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG12	9	1.2
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG13	9	1.2
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG21	9	1.2
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG22	9	1.2
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG23	9	1.2
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	3	1.2
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	3	1.2
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	3	1.2
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	3	1.2
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	3	1.2
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	3	1.2
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	3	1.2
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	3	1.2
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	3	1.2
(1,330)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	4	1.2
(1,330)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	4	1.2
(1,73)	1:6:A:ARG:HD2	1:7:A:LEU:H	5	1.2
(3,383)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	1.19
(2,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	1.19
(1,465)	1:3:A:GLU:HA	1:6:A:ARG:HB3	10	1.19
(1,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	1	1.19
(1,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	9	1.19
(1,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	10	1.19
(1,330)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	1	1.19
(1,330)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	1	1.19
(1,127)	1:10:A:GLN:HA	1:10:A:GLN:HG2	10	1.19
(3,383)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	1.18
(3,383)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	1.18
(3,280)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	1.18
(2,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	1.18
(2,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	1.18
(2,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	1.18
(1,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	9	1.18
(1,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	9	1.18
(1,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	9	1.18
(1,330)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	2	1.18
(1,330)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	2	1.18
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE2	1	1.18
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE3	1	1.18
(1,127)	1:10:A:GLN:HA	1:10:A:GLN:HG2	7	1.18
(1,58)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	9	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG11	6	1.17
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG12	6	1.17
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG13	6	1.17
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG21	6	1.17
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG22	6	1.17
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG23	6	1.17
(1,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	1	1.17
(1,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	7	1.17
(1,330)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	5	1.17
(1,330)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	5	1.17
(4,39)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	4	1.16
(4,39)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	4	1.16
(4,39)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	5	1.16
(4,39)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	5	1.16
(3,428)	1:5:A:VAL:HG21	1:6:A:ARG:HA	1	1.16
(3,428)	1:5:A:VAL:HG22	1:6:A:ARG:HA	1	1.16
(3,428)	1:5:A:VAL:HG23	1:6:A:ARG:HA	1	1.16
(2,468)	1:5:A:VAL:HG21	1:6:A:ARG:HA	1	1.16
(2,468)	1:5:A:VAL:HG22	1:6:A:ARG:HA	1	1.16
(2,468)	1:5:A:VAL:HG23	1:6:A:ARG:HA	1	1.16
(2,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	4	1.16
(2,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	4	1.16
(2,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	5	1.16
(2,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	5	1.16
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	3	1.16
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	3	1.16
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	3	1.16
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	3	1.16
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	3	1.16
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	3	1.16
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	3	1.16
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	3	1.16
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	3	1.16
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	3	1.16
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	3	1.16
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	3	1.16
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	3	1.16
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	3	1.16
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	3	1.16
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	3	1.16
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	3	1.16
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	3	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	2	1.16
(1,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	5	1.16
(3,280)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	1.15
(3,280)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	1.15
(2,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	1.15
(2,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	1.15
(1,404)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	2	1.15
(1,404)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	2	1.15
(1,404)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	2	1.15
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	7	1.15
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	7	1.15
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	7	1.15
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	7	1.15
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	7	1.15
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	7	1.15
(1,318)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	1	1.15
(3,383)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	1.14
(2,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	1.14
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	9	1.14
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	9	1.14
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	9	1.14
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	9	1.14
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	9	1.14
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	9	1.14
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	9	1.14
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	9	1.14
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	9	1.14
(1,404)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	4	1.14
(1,404)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	4	1.14
(1,404)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	4	1.14
(1,318)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	2	1.14
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	5	1.13
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	5	1.13
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	5	1.13
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	5	1.13
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	5	1.13
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	5	1.13
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	8	1.13
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	8	1.13
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	8	1.13
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	5	1.13
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	5	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	5	1.13
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	5	1.13
(1,58)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	10	1.13
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	7	1.12
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	7	1.12
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	7	1.12
(3,383)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	1.12
(3,280)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	1.12
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	7	1.12
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	7	1.12
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	7	1.12
(2,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	1.12
(2,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	1.12
(1,465)	1:3:A:GLU:HA	1:6:A:ARG:HB3	4	1.12
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE2	9	1.12
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE3	9	1.12
(1,32)	1:3:A:GLU:H	1:4:A:ALA:H	7	1.12
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	6	1.11
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	6	1.11
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	6	1.11
(4,33)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	1	1.11
(4,33)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	1	1.11
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	6	1.11
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	6	1.11
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	6	1.11
(2,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	1	1.11
(2,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	1	1.11
(1,404)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	3	1.11
(1,404)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	3	1.11
(1,404)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	3	1.11
(1,396)	1:12:A:LEU:HD21	1:17:A:PRO:HD3	7	1.11
(1,396)	1:12:A:LEU:HD22	1:17:A:PRO:HD3	7	1.11
(1,396)	1:12:A:LEU:HD23	1:17:A:PRO:HD3	7	1.11
(1,431)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	6	1.1
(1,431)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	6	1.1
(1,431)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	6	1.1
(1,396)	1:12:A:LEU:HD21	1:17:A:PRO:HD3	6	1.1
(1,396)	1:12:A:LEU:HD22	1:17:A:PRO:HD3	6	1.1
(1,396)	1:12:A:LEU:HD23	1:17:A:PRO:HD3	6	1.1
(1,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	7	1.1
(1,367)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	5	1.1
(1,367)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	5	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,39)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	2	1.09
(4,39)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	2	1.09
(2,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	2	1.09
(2,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	2	1.09
(1,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	9	1.09
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	10	1.09
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	10	1.09
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	10	1.09
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	10	1.09
(1,465)	1:3:A:GLU:HA	1:6:A:ARG:HB3	2	1.08
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	3	1.08
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	3	1.08
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	3	1.08
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	3	1.08
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	3	1.08
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	3	1.08
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	3	1.08
(1,58)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	1	1.08
(3,280)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	1.07
(2,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	1.07
(1,408)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	9	1.07
(1,396)	1:12:A:LEU:HD21	1:17:A:PRO:HD3	3	1.07
(1,396)	1:12:A:LEU:HD22	1:17:A:PRO:HD3	3	1.07
(1,396)	1:12:A:LEU:HD23	1:17:A:PRO:HD3	3	1.07
(1,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	3	1.07
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	1	1.06
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	1	1.06
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	1	1.06
(3,383)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	1.06
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	1	1.06
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	1	1.06
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	1	1.06
(2,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	1.06
(1,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	4	1.06
(1,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	4	1.06
(1,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	4	1.06
(1,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	4	1.06
(1,330)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	8	1.06
(1,330)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	8	1.06
(1,330)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	10	1.06
(1,330)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	10	1.06
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	1.05
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	1.05
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	1.05
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	1.05
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	1.05
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	10	1.05
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	10	1.05
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	10	1.05
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	10	1.05
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	10	1.05
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	10	1.05
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	10	1.05
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	10	1.05
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	10	1.05
(1,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	5	1.05
(1,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	9	1.05
(1,319)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	9	1.05
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	2	1.05
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	2	1.05
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	2	1.05
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	2	1.05
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	2	1.05
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	2	1.05
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	2	1.05
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	2	1.05
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	2	1.05
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	2	1.05
(1,32)	1:3:A:GLU:H	1:4:A:ALA:H	5	1.05
(1,32)	1:3:A:GLU:H	1:4:A:ALA:H	10	1.05
(3,383)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	1.04
(2,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	1.04
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB1	10	1.04
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB2	10	1.04
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB3	10	1.04
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB1	10	1.04
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB2	10	1.04
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB3	10	1.04
(1,404)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	1	1.04
(1,404)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	1	1.04
(1,404)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	1	1.04
(1,356)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	5	1.04
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	4	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	4	1.04
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	4	1.04
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	4	1.04
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	6	1.04
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	6	1.04
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	6	1.04
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	6	1.04
(1,58)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	8	1.04
(4,30)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	3	1.03
(3,70)	1:6:A:ARG:HB2	1:7:A:LEU:H	2	1.03
(3,70)	1:6:A:ARG:HB2	1:7:A:LEU:H	4	1.03
(2,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	3	1.03
(2,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	2	1.03
(2,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	4	1.03
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG2	8	1.03
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG2	8	1.03
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG2	8	1.03
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG3	8	1.03
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG3	8	1.03
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG3	8	1.03
(1,416)	1:8:A:TYR:HB2	1:24:A:PRO:HD2	10	1.03
(1,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	4	1.03
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	1	1.03
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	1	1.03
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	1	1.03
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	1	1.03
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG11	7	1.02
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG12	7	1.02
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG13	7	1.02
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG21	7	1.02
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG22	7	1.02
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG23	7	1.02
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	2	1.02
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	2	1.02
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	2	1.02
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	2	1.02
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	2	1.02
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	2	1.02
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	2	1.02
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	2	1.02
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	2	1.02
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	5	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	5	1.02
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	5	1.02
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	5	1.02
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	5	1.02
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	5	1.02
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	5	1.02
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	5	1.02
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	5	1.02
(1,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	2	1.02
(1,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	2	1.02
(1,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	2	1.02
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD2	1	1.02
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD3	1	1.02
(1,58)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	4	1.02
(3,370)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	1	1.01
(3,370)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	1	1.01
(3,370)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	1	1.01
(3,70)	1:6:A:ARG:HB2	1:7:A:LEU:H	8	1.01
(2,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	1	1.01
(2,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	1	1.01
(2,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	1	1.01
(2,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	8	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG11	2	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG12	2	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG13	2	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG21	2	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG22	2	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG23	2	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG11	4	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG12	4	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG13	4	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG21	4	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG22	4	1.01
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG23	4	1.01
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	1	1.01
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	1	1.01
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	1	1.01
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	1	1.01
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	1	1.01
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	1	1.01
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	1	1.01
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	1	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	1	1.01
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	5	1.01
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	5	1.01
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	5	1.01
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	5	1.01
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	5	1.01
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	5	1.01
(1,330)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	9	1.01
(1,330)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	9	1.01
(4,31)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	8	1.0
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD2	1	1.0
(3,70)	1:6:A:ARG:HB2	1:7:A:LEU:H	1	1.0
(2,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	8	1.0
(2,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	1	1.0
(2,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	1	1.0
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	7	1.0
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	7	1.0
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	7	1.0
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	7	1.0
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	7	1.0
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	7	1.0
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	7	1.0
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	7	1.0
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	7	1.0
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	7	1.0
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	7	1.0
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	7	1.0
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	7	1.0
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	7	1.0
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	7	1.0
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	7	1.0
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	7	1.0
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	7	1.0
(1,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	1	1.0
(1,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	1	1.0
(1,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	1	1.0
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD2	4	1.0
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD3	4	1.0
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	6	1.0
(1,58)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	2	1.0
(1,32)	1:3:A:GLU:H	1:4:A:ALA:H	4	1.0
(1,28)	1:3:A:GLU:HB3	1:4:A:ALA:H	3	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,29)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	5	0.99
(4,29)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	5	0.99
(4,29)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	5	0.99
(3,421)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	2	0.99
(3,421)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	5	0.99
(3,421)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	9	0.99
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	7	0.99
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	7	0.99
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	7	0.99
(2,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	2	0.99
(2,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	5	0.99
(2,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	9	0.99
(2,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	5	0.99
(2,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	5	0.99
(2,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	5	0.99
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	7	0.99
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	7	0.99
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	7	0.99
(1,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	0.99
(1,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	0.99
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	4	0.99
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	4	0.99
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	4	0.99
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	4	0.99
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	4	0.99
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	4	0.99
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	4	0.99
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	4	0.99
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	4	0.99
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	4	0.99
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	4	0.99
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	4	0.99
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	4	0.99
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	4	0.99
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	4	0.99
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	4	0.99
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	4	0.99
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	4	0.99
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	4	0.99
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	4	0.99
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	4	0.99
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	4	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	4	0.99
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	4	0.99
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	4	0.99
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	4	0.99
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	4	0.99
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	8	0.99
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	8	0.99
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	8	0.99
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	8	0.99
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	8	0.99
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	8	0.99
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	8	0.99
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	8	0.99
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	8	0.99
(1,404)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	5	0.99
(1,404)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	5	0.99
(1,404)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	5	0.99
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	9	0.98
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	9	0.98
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	9	0.98
(4,29)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	6	0.98
(4,29)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	6	0.98
(4,29)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	6	0.98
(4,29)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	9	0.98
(4,29)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	9	0.98
(4,29)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	9	0.98
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD2	9	0.98
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.98
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	5	0.98
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	5	0.98
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	5	0.98
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	6	0.98
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	6	0.98
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	6	0.98
(3,70)	1:6:A:ARG:HB2	1:7:A:LEU:H	9	0.98
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	5	0.98
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	5	0.98
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	5	0.98
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	9	0.98
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	9	0.98
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	9	0.98
(2,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	6	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	6	0.98
(2,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	6	0.98
(2,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	9	0.98
(2,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	9	0.98
(2,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	9	0.98
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	6	0.98
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	6	0.98
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	6	0.98
(2,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	9	0.98
(2,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.98
(2,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	9	0.98
(1,404)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	9	0.98
(1,404)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	9	0.98
(1,404)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	9	0.98
(1,318)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	8	0.98
(1,32)	1:3:A:GLU:H	1:4:A:ALA:H	8	0.98
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD2	4	0.97
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD2	5	0.97
(3,421)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	4	0.97
(2,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	4	0.97
(2,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	4	0.97
(2,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	5	0.97
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	2	0.97
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	2	0.97
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	2	0.97
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	2	0.97
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	2	0.97
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	2	0.97
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	2	0.97
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	2	0.97
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	2	0.97
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	2	0.97
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	2	0.97
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	2	0.97
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	2	0.97
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	2	0.97
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	2	0.97
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	2	0.97
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	2	0.97
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	2	0.97
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	5	0.97
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	5	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	5	0.97
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	5	0.97
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	5	0.97
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	5	0.97
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	5	0.97
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	5	0.97
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	5	0.97
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	5	0.97
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	5	0.97
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	5	0.97
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	5	0.97
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	5	0.97
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	5	0.97
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	5	0.97
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	5	0.97
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	5	0.97
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	10	0.97
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	10	0.97
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	10	0.97
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	10	0.97
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	10	0.97
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	10	0.97
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	10	0.97
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	10	0.97
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	10	0.97
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	10	0.97
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	10	0.97
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	10	0.97
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	10	0.97
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	10	0.97
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	10	0.97
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	10	0.97
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	10	0.97
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	10	0.97
(1,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	5	0.97
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	3	0.97
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	3	0.97
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	3	0.97
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	3	0.97
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	3	0.97
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	3	0.97
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	10	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	10	0.97
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	10	0.97
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	10	0.97
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	10	0.97
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	10	0.97
(1,318)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	4	0.97
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD2	3	0.97
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD3	3	0.97
(1,32)	1:3:A:GLU:H	1:4:A:ALA:H	9	0.97
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	4	0.96
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	4	0.96
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	4	0.96
(3,421)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	1	0.96
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	7	0.96
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	7	0.96
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	7	0.96
(2,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	1	0.96
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	7	0.96
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	7	0.96
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	7	0.96
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	4	0.96
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	4	0.96
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	4	0.96
(1,465)	1:3:A:GLU:HA	1:6:A:ARG:HB3	9	0.96
(1,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	3	0.96
(1,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	3	0.96
(1,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	5	0.96
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	1	0.96
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	1	0.96
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	1	0.96
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	1	0.96
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	1	0.96
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	1	0.96
(1,54)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	3	0.96
(1,47)	1:5:A:VAL:HG11	1:6:A:ARG:H	10	0.96
(1,47)	1:5:A:VAL:HG12	1:6:A:ARG:H	10	0.96
(1,47)	1:5:A:VAL:HG13	1:6:A:ARG:H	10	0.96
(1,47)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.96
(1,47)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.96
(1,47)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.96
(4,32)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	10	0.95
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD2	8	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	0.95
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	0.95
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	0.95
(3,442)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	1	0.95
(3,442)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	1	0.95
(3,442)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	1	0.95
(3,442)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	1	0.95
(3,442)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	1	0.95
(3,442)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	1	0.95
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	10	0.95
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	10	0.95
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	10	0.95
(3,381)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	10	0.95
(3,370)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	4	0.95
(3,370)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	4	0.95
(3,370)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	4	0.95
(2,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	1	0.95
(2,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	1	0.95
(2,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	1	0.95
(2,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	1	0.95
(2,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	1	0.95
(2,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	1	0.95
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	10	0.95
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	10	0.95
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	10	0.95
(2,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	10	0.95
(2,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	10	0.95
(2,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	4	0.95
(2,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	4	0.95
(2,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	4	0.95
(2,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	8	0.95
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	0.95
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	0.95
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	0.95
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG2	3	0.95
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG2	3	0.95
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG2	3	0.95
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG3	3	0.95
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG3	3	0.95
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG3	3	0.95
(1,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	1	0.95
(1,318)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	5	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	4	0.95
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	4	0.95
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	4	0.95
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	4	0.95
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	4	0.95
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	4	0.95
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HG	7	0.95
(1,47)	1:5:A:VAL:HG11	1:6:A:ARG:H	5	0.95
(1,47)	1:5:A:VAL:HG12	1:6:A:ARG:H	5	0.95
(1,47)	1:5:A:VAL:HG13	1:6:A:ARG:H	5	0.95
(1,47)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	0.95
(1,47)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	0.95
(1,47)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	0.95
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	2	0.94
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	2	0.94
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	2	0.94
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD2	2	0.94
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD2	3	0.94
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD2	6	0.94
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD2	7	0.94
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	2	0.94
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	2	0.94
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	2	0.94
(2,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	2	0.94
(2,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	3	0.94
(2,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	6	0.94
(2,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	7	0.94
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG11	10	0.94
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG12	10	0.94
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG13	10	0.94
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG21	10	0.94
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG22	10	0.94
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG23	10	0.94
(1,404)	1:7:A:LEU:HD11	1:8:A:TYR:HB3	6	0.94
(1,404)	1:7:A:LEU:HD12	1:8:A:TYR:HB3	6	0.94
(1,404)	1:7:A:LEU:HD13	1:8:A:TYR:HB3	6	0.94
(1,318)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	9	0.94
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	7	0.94
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	7	0.94
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	7	0.94
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	7	0.94
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	7	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	7	0.94
(1,60)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	7	0.94
(4,29)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	1	0.93
(4,29)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	1	0.93
(4,29)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	1	0.93
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.93
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.93
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.93
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.93
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.93
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.93
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.93
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.93
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.93
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	4	0.93
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	4	0.93
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	4	0.93
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	5	0.93
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	5	0.93
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	5	0.93
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	4	0.93
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	4	0.93
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	4	0.93
(2,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	1	0.93
(2,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	1	0.93
(2,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	1	0.93
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	5	0.93
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	5	0.93
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	5	0.93
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.93
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.93
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.93
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.93
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.93
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.93
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.93
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.93
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.93
(1,318)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	10	0.93
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	8	0.93
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HG	5	0.93
(1,54)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	2	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	8	0.93
(1,54)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.93
(1,47)	1:5:A:VAL:HG11	1:6:A:ARG:H	9	0.93
(1,47)	1:5:A:VAL:HG12	1:6:A:ARG:H	9	0.93
(1,47)	1:5:A:VAL:HG13	1:6:A:ARG:H	9	0.93
(1,47)	1:5:A:VAL:HG21	1:6:A:ARG:H	9	0.93
(1,47)	1:5:A:VAL:HG22	1:6:A:ARG:H	9	0.93
(1,47)	1:5:A:VAL:HG23	1:6:A:ARG:H	9	0.93
(1,32)	1:3:A:GLU:H	1:4:A:ALA:H	1	0.93
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.92
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.92
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.92
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.92
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.92
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.92
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.92
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.92
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.92
(3,421)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	6	0.92
(3,394)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	9	0.92
(3,393)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	10	0.92
(3,168)	1:13:A:LYS:H	1:13:A:LYS:HB3	7	0.92
(2,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	6	0.92
(2,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	9	0.92
(2,427)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	10	0.92
(2,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	7	0.92
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.92
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.92
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.92
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.92
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.92
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.92
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.92
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.92
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.92
(1,330)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	6	0.92
(1,330)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	6	0.92
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	7	0.92
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	7	0.92
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	7	0.92
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD2	8	0.92
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD3	8	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB3	2	0.92
(1,32)	1:3:A:GLU:H	1:4:A:ALA:H	2	0.92
(4,41)	1:13:A:LYS:H	1:14:A:GLN:HA	10	0.91
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	8	0.91
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	8	0.91
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	8	0.91
(4,28)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	6	0.91
(4,28)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	6	0.91
(4,28)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	6	0.91
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.91
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.91
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.91
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	1	0.91
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	1	0.91
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	1	0.91
(2,472)	1:13:A:LYS:H	1:14:A:GLN:HA	10	0.91
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	1	0.91
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	1	0.91
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	1	0.91
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	8	0.91
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	8	0.91
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	8	0.91
(2,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	6	0.91
(2,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	6	0.91
(2,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	6	0.91
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.91
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.91
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.91
(1,408)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	5	0.91
(1,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	3	0.91
(1,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	3	0.91
(1,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	3	0.91
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB3	4	0.91
(1,54)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	4	0.91
(4,41)	1:13:A:LYS:H	1:14:A:GLN:HA	8	0.9
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.9
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.9
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.9
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	2	0.9
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	2	0.9
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	2	0.9
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	9	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	9	0.9
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	9	0.9
(3,370)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	2	0.9
(3,370)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	2	0.9
(3,370)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	2	0.9
(2,472)	1:13:A:LYS:H	1:14:A:GLN:HA	8	0.9
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	2	0.9
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	2	0.9
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	2	0.9
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	9	0.9
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	9	0.9
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	9	0.9
(2,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	2	0.9
(2,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	2	0.9
(2,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	2	0.9
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.9
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.9
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.9
(1,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	7	0.9
(1,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	7	0.9
(1,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	7	0.9
(1,347)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	3	0.9
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB3	1	0.9
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB3	3	0.9
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB3	8	0.9
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB3	9	0.9
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	2	0.9
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	3	0.9
(1,54)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	1	0.9
(1,54)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	9	0.9
(1,47)	1:5:A:VAL:HG11	1:6:A:ARG:H	3	0.9
(1,47)	1:5:A:VAL:HG12	1:6:A:ARG:H	3	0.9
(1,47)	1:5:A:VAL:HG13	1:6:A:ARG:H	3	0.9
(1,47)	1:5:A:VAL:HG21	1:6:A:ARG:H	3	0.9
(1,47)	1:5:A:VAL:HG22	1:6:A:ARG:H	3	0.9
(1,47)	1:5:A:VAL:HG23	1:6:A:ARG:H	3	0.9
(1,47)	1:5:A:VAL:HG11	1:6:A:ARG:H	6	0.9
(1,47)	1:5:A:VAL:HG12	1:6:A:ARG:H	6	0.9
(1,47)	1:5:A:VAL:HG13	1:6:A:ARG:H	6	0.9
(1,47)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.9
(1,47)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.9
(1,47)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,28)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	3	0.89
(4,28)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	3	0.89
(4,28)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	3	0.89
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.89
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.89
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.89
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	3	0.89
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	3	0.89
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	3	0.89
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	3	0.89
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	3	0.89
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	3	0.89
(2,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	3	0.89
(2,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	3	0.89
(2,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	3	0.89
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.89
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.89
(2,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.89
(1,465)	1:3:A:GLU:HA	1:6:A:ARG:HB3	8	0.89
(1,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	8	0.89
(1,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	8	0.89
(1,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	5	0.89
(1,409)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	6	0.89
(1,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	2	0.89
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB3	5	0.89
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.89
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	4	0.89
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	9	0.89
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HG	3	0.89
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HG	4	0.89
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HG	6	0.89
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HG	8	0.89
(1,60)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	6	0.89
(1,47)	1:5:A:VAL:HG11	1:6:A:ARG:H	8	0.89
(1,47)	1:5:A:VAL:HG12	1:6:A:ARG:H	8	0.89
(1,47)	1:5:A:VAL:HG13	1:6:A:ARG:H	8	0.89
(1,47)	1:5:A:VAL:HG21	1:6:A:ARG:H	8	0.89
(1,47)	1:5:A:VAL:HG22	1:6:A:ARG:H	8	0.89
(1,47)	1:5:A:VAL:HG23	1:6:A:ARG:H	8	0.89
(3,421)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	10	0.88
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	10	0.88
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	10	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	10	0.88
(3,364)	1:9:A:ILE:HA	1:12:A:LEU:HB3	1	0.88
(3,364)	1:9:A:ILE:HA	1:12:A:LEU:HB3	5	0.88
(2,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	10	0.88
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	10	0.88
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	10	0.88
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	10	0.88
(2,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	1	0.88
(2,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	5	0.88
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG11	5	0.88
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG12	5	0.88
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG13	5	0.88
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG21	5	0.88
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG22	5	0.88
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG23	5	0.88
(1,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	6	0.88
(1,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	6	0.88
(1,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	6	0.88
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	5	0.88
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	5	0.88
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	5	0.88
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	5	0.88
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	5	0.88
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	5	0.88
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB3	6	0.88
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB3	7	0.88
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	1	0.88
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	5	0.88
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HG	1	0.88
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HG	2	0.88
(1,60)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	5	0.88
(1,32)	1:3:A:GLU:H	1:4:A:ALA:H	6	0.88
(4,28)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	7	0.87
(4,28)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	7	0.87
(4,28)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	7	0.87
(3,364)	1:9:A:ILE:HA	1:12:A:LEU:HB3	2	0.87
(3,364)	1:9:A:ILE:HA	1:12:A:LEU:HB3	4	0.87
(2,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	7	0.87
(2,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	7	0.87
(2,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	7	0.87
(2,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	2	0.87
(2,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	4	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	9	0.87
(1,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	9	0.87
(1,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	1	0.87
(1,356)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.87
(1,332)	1:12:A:LEU:H	1:12:A:LEU:HG	5	0.87
(1,188)	1:14:A:GLN:H	1:14:A:GLN:HG3	3	0.87
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.87
(1,45)	1:5:A:VAL:H	1:6:A:ARG:H	3	0.87
(3,364)	1:9:A:ILE:HA	1:12:A:LEU:HB3	9	0.86
(3,325)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	8	0.86
(2,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	9	0.86
(2,347)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	8	0.86
(1,343)	1:10:A:GLN:HE21	1:14:A:GLN:HG3	1	0.86
(1,332)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.86
(1,332)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.86
(1,332)	1:12:A:LEU:H	1:12:A:LEU:HG	4	0.86
(1,332)	1:12:A:LEU:H	1:12:A:LEU:HG	6	0.86
(1,330)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	3	0.86
(1,330)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	3	0.86
(1,187)	1:14:A:GLN:H	1:14:A:GLN:HG2	9	0.86
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HG	9	0.86
(1,47)	1:5:A:VAL:HG11	1:6:A:ARG:H	2	0.86
(1,47)	1:5:A:VAL:HG12	1:6:A:ARG:H	2	0.86
(1,47)	1:5:A:VAL:HG13	1:6:A:ARG:H	2	0.86
(1,47)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	0.86
(1,47)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	0.86
(1,47)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	0.86
(1,45)	1:5:A:VAL:H	1:6:A:ARG:H	2	0.86
(3,370)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	10	0.85
(3,370)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	10	0.85
(3,370)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	10	0.85
(3,364)	1:9:A:ILE:HA	1:12:A:LEU:HB3	10	0.85
(2,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	10	0.85
(2,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	10	0.85
(2,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	10	0.85
(2,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	10	0.85
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG2	7	0.85
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG2	7	0.85
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG2	7	0.85
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG3	7	0.85
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG3	7	0.85
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG3	7	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD2	10	0.85
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD3	10	0.85
(1,131)	1:10:A:GLN:HB2	1:10:A:GLN:HE21	7	0.85
(1,131)	1:10:A:GLN:HB3	1:10:A:GLN:HE21	7	0.85
(3,394)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	2	0.84
(2,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	2	0.84
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG2	6	0.84
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG2	6	0.84
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG2	6	0.84
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG3	6	0.84
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG3	6	0.84
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG3	6	0.84
(1,382)	1:10:A:GLN:HA	1:13:A:LYS:HG2	10	0.84
(1,382)	1:10:A:GLN:HA	1:13:A:LYS:HG3	10	0.84
(1,319)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	3	0.84
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD11	3	0.84
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD12	3	0.84
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD13	3	0.84
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD11	9	0.84
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD12	9	0.84
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD13	9	0.84
(1,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	7	0.84
(1,7)	1:19:A:SER:H	1:19:A:SER:HA	8	0.84
(1,7)	1:19:A:SER:H	1:19:A:SER:HA	10	0.84
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.83
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.83
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.83
(3,421)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	7	0.83
(3,168)	1:13:A:LYS:H	1:13:A:LYS:HB3	8	0.83
(3,134)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.83
(2,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	7	0.83
(2,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	8	0.83
(2,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.83
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.83
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.83
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.83
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG2	1	0.83
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG2	1	0.83
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG2	1	0.83
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG3	1	0.83
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG3	1	0.83
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG3	1	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG2	2	0.83
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG2	2	0.83
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG2	2	0.83
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG3	2	0.83
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG3	2	0.83
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG3	2	0.83
(1,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	8	0.83
(1,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	8	0.83
(1,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	8	0.83
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	1	0.83
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	1	0.83
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	1	0.83
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	10	0.83
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	10	0.83
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	10	0.83
(1,117)	1:9:A:ILE:H	1:9:A:ILE:HG13	7	0.83
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD11	10	0.83
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD12	10	0.83
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD13	10	0.83
(1,47)	1:5:A:VAL:HG11	1:6:A:ARG:H	4	0.83
(1,47)	1:5:A:VAL:HG12	1:6:A:ARG:H	4	0.83
(1,47)	1:5:A:VAL:HG13	1:6:A:ARG:H	4	0.83
(1,47)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	0.83
(1,47)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	0.83
(1,47)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	0.83
(1,45)	1:5:A:VAL:H	1:6:A:ARG:H	10	0.83
(1,7)	1:19:A:SER:H	1:19:A:SER:HA	5	0.83
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD11	5	0.82
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD12	5	0.82
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD13	5	0.82
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD11	7	0.82
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD12	7	0.82
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD13	7	0.82
(3,134)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.82
(3,134)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.82
(3,134)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.82
(3,134)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	0.82
(2,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.82
(2,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.82
(2,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.82
(2,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	0.82
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	5	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	5	0.82
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	5	0.82
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	7	0.82
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	7	0.82
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	7	0.82
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB1	9	0.82
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB2	9	0.82
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB3	9	0.82
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB1	9	0.82
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB2	9	0.82
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB3	9	0.82
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG2	5	0.82
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG2	5	0.82
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG2	5	0.82
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG3	5	0.82
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG3	5	0.82
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG3	5	0.82
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	9	0.82
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	9	0.82
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	9	0.82
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	9	0.82
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	9	0.82
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	9	0.82
(1,347)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	4	0.82
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD2	5	0.82
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD3	5	0.82
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD2	7	0.82
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD3	7	0.82
(1,117)	1:9:A:ILE:H	1:9:A:ILE:HG13	8	0.82
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD11	4	0.82
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD12	4	0.82
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD13	4	0.82
(1,47)	1:5:A:VAL:HG11	1:6:A:ARG:H	7	0.82
(1,47)	1:5:A:VAL:HG12	1:6:A:ARG:H	7	0.82
(1,47)	1:5:A:VAL:HG13	1:6:A:ARG:H	7	0.82
(1,47)	1:5:A:VAL:HG21	1:6:A:ARG:H	7	0.82
(1,47)	1:5:A:VAL:HG22	1:6:A:ARG:H	7	0.82
(1,47)	1:5:A:VAL:HG23	1:6:A:ARG:H	7	0.82
(1,45)	1:5:A:VAL:H	1:6:A:ARG:H	4	0.82
(4,29)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	4	0.81
(4,29)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	4	0.81
(4,29)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	4	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,134)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.81
(3,134)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	0.81
(3,134)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.81
(2,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	4	0.81
(2,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	4	0.81
(2,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	4	0.81
(2,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.81
(2,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	0.81
(2,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.81
(1,441)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	6	0.81
(1,441)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	6	0.81
(1,441)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	6	0.81
(1,408)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	2	0.81
(1,408)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	10	0.81
(1,332)	1:12:A:LEU:H	1:12:A:LEU:HG	7	0.81
(1,332)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.81
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	7	0.81
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG3	7	0.81
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	8	0.81
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	8	0.81
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	8	0.81
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	8	0.81
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG2	9	0.81
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG3	9	0.81
(3,317)	1:10:A:GLN:HB2	1:11:A:TRP:H	5	0.8
(3,317)	1:10:A:GLN:HB2	1:11:A:TRP:H	9	0.8
(3,134)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.8
(3,134)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.8
(2,339)	1:10:A:GLN:HB2	1:11:A:TRP:H	5	0.8
(2,339)	1:10:A:GLN:HB2	1:11:A:TRP:H	9	0.8
(2,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.8
(2,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.8
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG2	4	0.8
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG2	4	0.8
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG2	4	0.8
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG3	4	0.8
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG3	4	0.8
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG3	4	0.8
(1,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	7	0.8
(1,408)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	6	0.8
(1,347)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	2	0.8
(1,187)	1:14:A:GLN:H	1:14:A:GLN:HG2	10	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:10:A:GLN:HB2	1:10:A:GLN:HE21	10	0.8
(1,131)	1:10:A:GLN:HB3	1:10:A:GLN:HE21	10	0.8
(1,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	6	0.8
(4,29)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	3	0.79
(4,29)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	3	0.79
(4,29)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	3	0.79
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.79
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.79
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD11	4	0.79
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD12	4	0.79
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD13	4	0.79
(3,382)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	3	0.79
(3,382)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	10	0.79
(3,370)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	5	0.79
(3,370)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	5	0.79
(3,370)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	5	0.79
(3,317)	1:10:A:GLN:HB2	1:11:A:TRP:H	8	0.79
(3,70)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.79
(2,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	3	0.79
(2,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	10	0.79
(2,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	3	0.79
(2,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	3	0.79
(2,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	3	0.79
(2,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	5	0.79
(2,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	5	0.79
(2,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	5	0.79
(2,339)	1:10:A:GLN:HB2	1:11:A:TRP:H	8	0.79
(2,92)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.79
(2,92)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.79
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	4	0.79
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	4	0.79
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	4	0.79
(2,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.79
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB1	5	0.79
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB2	5	0.79
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB3	5	0.79
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB1	5	0.79
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB2	5	0.79
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB3	5	0.79
(1,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	6	0.79
(1,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	6	0.79
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG2	10	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG2	10	0.79
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG2	10	0.79
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG3	10	0.79
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG3	10	0.79
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG3	10	0.79
(1,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	7	0.79
(1,347)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	9	0.79
(1,314)	1:8:A:TYR:HD1	1:9:A:ILE:H	10	0.79
(1,314)	1:8:A:TYR:HD2	1:9:A:ILE:H	10	0.79
(1,194)	1:18:A:SER:H	1:18:A:SER:HB2	3	0.79
(1,194)	1:18:A:SER:H	1:18:A:SER:HB3	3	0.79
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG2	1	0.79
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG3	1	0.79
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD11	2	0.79
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD12	2	0.79
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD13	2	0.79
(1,45)	1:5:A:VAL:H	1:6:A:ARG:H	1	0.79
(1,45)	1:5:A:VAL:H	1:6:A:ARG:H	8	0.79
(1,45)	1:5:A:VAL:H	1:6:A:ARG:H	9	0.79
(4,29)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	2	0.78
(4,29)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	2	0.78
(4,29)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	2	0.78
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HB2	5	0.78
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.78
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD11	6	0.78
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD12	6	0.78
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD13	6	0.78
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.78
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.78
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.78
(3,394)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	5	0.78
(3,317)	1:10:A:GLN:HB2	1:11:A:TRP:H	1	0.78
(3,286)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	8	0.78
(2,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	5	0.78
(2,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	2	0.78
(2,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	2	0.78
(2,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	2	0.78
(2,339)	1:10:A:GLN:HB2	1:11:A:TRP:H	1	0.78
(2,306)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	8	0.78
(2,92)	1:7:A:LEU:H	1:7:A:LEU:HB2	5	0.78
(2,92)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.78
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	6	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	6	0.78
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	6	0.78
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.78
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.78
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.78
(1,416)	1:8:A:TYR:HB2	1:24:A:PRO:HD2	3	0.78
(1,356)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	8	0.78
(1,332)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.78
(1,239)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	4	0.78
(1,239)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	6	0.78
(1,239)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	8	0.78
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	8	0.78
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	8	0.78
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	8	0.78
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	8	0.78
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD11	1	0.78
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD12	1	0.78
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD13	1	0.78
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HB2	2	0.77
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.77
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.77
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.77
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HB2	7	0.77
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.77
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD11	8	0.77
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD12	8	0.77
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD13	8	0.77
(3,381)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	3	0.77
(3,317)	1:10:A:GLN:HB2	1:11:A:TRP:H	4	0.77
(2,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	3	0.77
(2,339)	1:10:A:GLN:HB2	1:11:A:TRP:H	4	0.77
(2,92)	1:7:A:LEU:H	1:7:A:LEU:HB2	2	0.77
(2,92)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.77
(2,92)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.77
(2,92)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.77
(2,92)	1:7:A:LEU:H	1:7:A:LEU:HB2	7	0.77
(2,92)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.77
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	8	0.77
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	8	0.77
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	8	0.77
(1,465)	1:3:A:GLU:HA	1:6:A:ARG:HB3	3	0.77
(1,408)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	4	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:14:A:GLN:HE21	1:14:A:GLN:HG3	2	0.77
(1,344)	1:14:A:GLN:HE21	1:14:A:GLN:HG3	6	0.77
(1,341)	1:21:A:ARG:H	1:21:A:ARG:HG2	7	0.77
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	4	0.77
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	4	0.77
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	4	0.77
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	6	0.77
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	6	0.77
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	6	0.77
(1,239)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	1	0.77
(1,239)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	2	0.77
(1,239)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	5	0.77
(1,239)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	7	0.77
(1,239)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	9	0.77
(1,187)	1:14:A:GLN:H	1:14:A:GLN:HG2	5	0.77
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG2	6	0.77
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG3	6	0.77
(1,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	5	0.77
(3,364)	1:9:A:ILE:HA	1:12:A:LEU:HB3	7	0.76
(3,317)	1:10:A:GLN:HB2	1:11:A:TRP:H	2	0.76
(3,286)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	1	0.76
(3,286)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	9	0.76
(3,286)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	10	0.76
(3,114)	1:10:A:GLN:H	1:10:A:GLN:HB2	8	0.76
(2,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	7	0.76
(2,339)	1:10:A:GLN:HB2	1:11:A:TRP:H	2	0.76
(2,306)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	1	0.76
(2,306)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	9	0.76
(2,306)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	10	0.76
(2,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	8	0.76
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG11	3	0.76
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG12	3	0.76
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG13	3	0.76
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG21	3	0.76
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG22	3	0.76
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG23	3	0.76
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	7	0.76
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	7	0.76
(1,449)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	7	0.76
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	7	0.76
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	7	0.76
(1,449)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	7	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	7	0.76
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	7	0.76
(1,449)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	7	0.76
(1,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	6	0.76
(1,332)	1:12:A:LEU:H	1:12:A:LEU:HG	3	0.76
(1,332)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.76
(1,239)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	3	0.76
(1,239)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	10	0.76
(1,194)	1:18:A:SER:H	1:18:A:SER:HB2	7	0.76
(1,194)	1:18:A:SER:H	1:18:A:SER:HB3	7	0.76
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD11	1	0.75
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD12	1	0.75
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD13	1	0.75
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.75
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.75
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.75
(3,394)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	1	0.75
(3,285)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.75
(2,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	1	0.75
(2,304)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.75
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD11	1	0.75
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD12	1	0.75
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD13	1	0.75
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.75
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.75
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.75
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD21	1	0.75
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD22	1	0.75
(1,452)	1:5:A:VAL:HG11	1:12:A:LEU:HD23	1	0.75
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD21	1	0.75
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD22	1	0.75
(1,452)	1:5:A:VAL:HG12	1:12:A:LEU:HD23	1	0.75
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD21	1	0.75
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD22	1	0.75
(1,452)	1:5:A:VAL:HG13	1:12:A:LEU:HD23	1	0.75
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD21	1	0.75
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD22	1	0.75
(1,452)	1:5:A:VAL:HG21	1:12:A:LEU:HD23	1	0.75
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD21	1	0.75
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD22	1	0.75
(1,452)	1:5:A:VAL:HG22	1:12:A:LEU:HD23	1	0.75
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD21	1	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD22	1	0.75
(1,452)	1:5:A:VAL:HG23	1:12:A:LEU:HD23	1	0.75
(1,444)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	1	0.75
(1,444)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	1	0.75
(1,444)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	1	0.75
(1,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	1	0.75
(1,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	1	0.75
(1,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	1	0.75
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	1	0.75
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	1	0.75
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	1	0.75
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	1	0.75
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	1	0.75
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	1	0.75
(1,347)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	10	0.75
(1,326)	1:11:A:TRP:HB3	1:12:A:LEU:H	2	0.75
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	2	0.75
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	2	0.75
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	2	0.75
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	9	0.75
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	9	0.75
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	9	0.75
(1,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	6	0.75
(1,194)	1:18:A:SER:H	1:18:A:SER:HB2	6	0.75
(1,194)	1:18:A:SER:H	1:18:A:SER:HB3	6	0.75
(1,187)	1:14:A:GLN:H	1:14:A:GLN:HG2	4	0.75
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG2	4	0.75
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG3	4	0.75
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD11	6	0.75
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD12	6	0.75
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD13	6	0.75
(1,72)	1:6:A:ARG:HD3	1:7:A:LEU:H	9	0.75
(4,41)	1:13:A:LYS:H	1:14:A:GLN:HA	7	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD11	2	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD12	2	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD13	2	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD11	5	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD12	5	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD13	5	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.74
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.74
(3,317)	1:10:A:GLN:HB2	1:11:A:TRP:H	3	0.74
(3,286)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	2	0.74
(3,285)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.74
(3,168)	1:13:A:LYS:H	1:13:A:LYS:HB3	1	0.74
(2,472)	1:13:A:LYS:H	1:14:A:GLN:HA	7	0.74
(2,339)	1:10:A:GLN:HB2	1:11:A:TRP:H	3	0.74
(2,306)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	2	0.74
(2,304)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.74
(2,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	1	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD11	2	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD12	2	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD13	2	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD11	5	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD12	5	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD13	5	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.74
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.74
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	8	0.74
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	8	0.74
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	8	0.74
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	8	0.74
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	8	0.74
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	8	0.74
(1,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	6	0.74
(1,388)	1:5:A:VAL:HA	1:8:A:TYR:HB3	10	0.74
(1,326)	1:11:A:TRP:HB3	1:12:A:LEU:H	5	0.74
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	5	0.74
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	5	0.74
(1,309)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	5	0.74
(1,256)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	0.74
(1,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	7	0.74
(1,186)	1:14:A:GLN:H	1:14:A:GLN:HB3	7	0.74
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG2	2	0.74
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG3	2	0.74
(4,28)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	8	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,28)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	8	0.73
(4,28)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	8	0.73
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD11	8	0.73
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD12	8	0.73
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD13	8	0.73
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.73
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.73
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.73
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.73
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.73
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.73
(3,360)	1:15:A:GLY:HA3	1:18:A:SER:HB3	10	0.73
(3,286)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	7	0.73
(3,70)	1:6:A:ARG:HB2	1:7:A:LEU:H	3	0.73
(2,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	8	0.73
(2,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	8	0.73
(2,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	8	0.73
(2,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	10	0.73
(2,306)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	7	0.73
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD11	8	0.73
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD12	8	0.73
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD13	8	0.73
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.73
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.73
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.73
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.73
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.73
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.73
(2,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	3	0.73
(1,465)	1:3:A:GLU:HA	1:6:A:ARG:HB3	1	0.73
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG2	9	0.73
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG2	9	0.73
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG2	9	0.73
(1,433)	1:12:A:LEU:HD21	1:17:A:PRO:HG3	9	0.73
(1,433)	1:12:A:LEU:HD22	1:17:A:PRO:HG3	9	0.73
(1,433)	1:12:A:LEU:HD23	1:17:A:PRO:HG3	9	0.73
(1,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	10	0.73
(1,416)	1:8:A:TYR:HB2	1:24:A:PRO:HD2	7	0.73
(1,117)	1:9:A:ILE:H	1:9:A:ILE:HG13	1	0.73
(1,45)	1:5:A:VAL:H	1:6:A:ARG:H	6	0.73
(3,394)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	4	0.72
(3,346)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	1	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,346)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	1	0.72
(3,346)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	1	0.72
(3,346)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	1	0.72
(3,346)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	1	0.72
(3,346)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	1	0.72
(3,286)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	3	0.72
(3,285)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.72
(2,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	4	0.72
(2,370)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	1	0.72
(2,370)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	1	0.72
(2,370)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	1	0.72
(2,370)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	1	0.72
(2,370)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	1	0.72
(2,370)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	1	0.72
(2,306)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	3	0.72
(2,304)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.72
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB1	2	0.72
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB2	2	0.72
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB3	2	0.72
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB1	2	0.72
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB2	2	0.72
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB3	2	0.72
(1,367)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	2	0.72
(1,367)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	2	0.72
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	6	0.72
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	6	0.72
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	6	0.72
(1,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	7	0.72
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG2	8	0.72
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG3	8	0.72
(1,117)	1:9:A:ILE:H	1:9:A:ILE:HG13	9	0.72
(1,117)	1:9:A:ILE:H	1:9:A:ILE:HG13	10	0.72
(4,41)	1:13:A:LYS:H	1:14:A:GLN:HA	9	0.71
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD11	3	0.71
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD12	3	0.71
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD13	3	0.71
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD11	7	0.71
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD12	7	0.71
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD13	7	0.71
(3,285)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.71
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	3	0.71
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	3	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	5	0.71
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	5	0.71
(2,472)	1:13:A:LYS:H	1:14:A:GLN:HA	9	0.71
(2,304)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.71
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	3	0.71
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	3	0.71
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	5	0.71
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	5	0.71
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD11	3	0.71
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD12	3	0.71
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD13	3	0.71
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD11	7	0.71
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD12	7	0.71
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD13	7	0.71
(1,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	4	0.71
(1,356)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	4	0.71
(1,341)	1:21:A:ARG:H	1:21:A:ARG:HG2	4	0.71
(1,329)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	6	0.71
(1,329)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	6	0.71
(1,326)	1:11:A:TRP:HB3	1:12:A:LEU:H	1	0.71
(1,326)	1:11:A:TRP:HB3	1:12:A:LEU:H	4	0.71
(1,326)	1:11:A:TRP:HB3	1:12:A:LEU:H	8	0.71
(1,326)	1:11:A:TRP:HB3	1:12:A:LEU:H	10	0.71
(1,319)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	5	0.71
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	9	0.71
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	9	0.71
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	9	0.71
(1,280)	1:21:A:ARG:HA	1:21:A:ARG:HG3	9	0.71
(1,117)	1:9:A:ILE:H	1:9:A:ILE:HG13	2	0.71
(1,117)	1:9:A:ILE:H	1:9:A:ILE:HG13	4	0.71
(1,117)	1:9:A:ILE:H	1:9:A:ILE:HG13	5	0.71
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD11	6	0.7
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD12	6	0.7
(4,10)	1:9:A:ILE:HA	1:9:A:ILE:HD13	6	0.7
(3,393)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	9	0.7
(3,363)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	6	0.7
(3,317)	1:10:A:GLN:HB2	1:11:A:TRP:H	6	0.7
(3,286)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	4	0.7
(3,286)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	5	0.7
(3,285)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.7
(2,427)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	9	0.7
(2,389)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	6	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,339)	1:10:A:GLN:HB2	1:11:A:TRP:H	6	0.7
(2,306)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	4	0.7
(2,306)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	5	0.7
(2,304)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.7
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD11	6	0.7
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD12	6	0.7
(2,105)	1:9:A:ILE:HA	1:9:A:ILE:HD13	6	0.7
(1,408)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	1	0.7
(1,388)	1:5:A:VAL:HA	1:8:A:TYR:HB3	3	0.7
(1,343)	1:10:A:GLN:HE21	1:14:A:GLN:HG3	3	0.7
(1,338)	1:21:A:ARG:H	1:21:A:ARG:HB2	10	0.7
(1,326)	1:11:A:TRP:HB3	1:12:A:LEU:H	3	0.7
(1,258)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	7	0.7
(1,258)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	8	0.7
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	1	0.7
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	1	0.7
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	1	0.7
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	1	0.7
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	1	0.7
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	1	0.7
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	1	0.7
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	1	0.7
(1,102)	1:9:A:ILE:HA	1:9:A:ILE:HG12	6	0.7
(1,54)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	5	0.7
(1,28)	1:3:A:GLU:HB3	1:4:A:ALA:H	2	0.7
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.69
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.69
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.69
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HG3	3	0.69
(3,363)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	7	0.69
(2,389)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	7	0.69
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.69
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.69
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.69
(2,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	3	0.69
(1,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	8	0.69
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.69
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	10	0.69
(1,326)	1:11:A:TRP:HB3	1:12:A:LEU:H	9	0.69
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	10	0.69
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	10	0.69
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	10	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	7	0.69
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	7	0.69
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	7	0.69
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	7	0.69
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	8	0.69
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	8	0.69
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	8	0.69
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	8	0.69
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	9	0.69
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	9	0.69
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	9	0.69
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	9	0.69
(1,117)	1:9:A:ILE:H	1:9:A:ILE:HG13	3	0.69
(1,45)	1:5:A:VAL:H	1:6:A:ARG:H	5	0.69
(1,45)	1:5:A:VAL:H	1:6:A:ARG:H	7	0.69
(4,15)	1:17:A:PRO:HA	1:17:A:PRO:HD3	2	0.68
(3,285)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.68
(3,285)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.68
(2,304)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.68
(2,304)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.68
(2,201)	1:17:A:PRO:HA	1:17:A:PRO:HD3	2	0.68
(1,416)	1:8:A:TYR:HB2	1:24:A:PRO:HD2	8	0.68
(1,367)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	1	0.68
(1,367)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	1	0.68
(1,354)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	10	0.68
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	4	0.68
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	4	0.68
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	4	0.68
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	7	0.68
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	7	0.68
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	7	0.68
(1,270)	1:24:A:PRO:HA	1:24:A:PRO:HG3	10	0.68
(1,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	8	0.68
(1,186)	1:14:A:GLN:H	1:14:A:GLN:HB3	8	0.68
(1,102)	1:9:A:ILE:HA	1:9:A:ILE:HG12	3	0.68
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD11	5	0.68
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD12	5	0.68
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD13	5	0.68
(1,54)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	6	0.68
(4,29)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	7	0.67
(4,29)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	7	0.67
(4,29)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	7	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,363)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	8	0.67
(3,285)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.67
(2,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	7	0.67
(2,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	7	0.67
(2,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	7	0.67
(2,389)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	8	0.67
(2,304)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.67
(1,444)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	7	0.67
(1,444)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	7	0.67
(1,444)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	7	0.67
(1,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	7	0.67
(1,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	7	0.67
(1,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	7	0.67
(1,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	6	0.67
(1,357)	1:11:A:TRP:HD1	1:23:A:PRO:HG3	8	0.67
(1,326)	1:11:A:TRP:HB3	1:12:A:LEU:H	6	0.67
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	2	0.67
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	2	0.67
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	2	0.67
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	5	0.67
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	5	0.67
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	5	0.67
(1,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	5	0.67
(1,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	0.67
(1,194)	1:18:A:SER:H	1:18:A:SER:HB2	5	0.67
(1,194)	1:18:A:SER:H	1:18:A:SER:HB3	5	0.67
(1,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	7	0.67
(1,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	8	0.67
(1,117)	1:9:A:ILE:H	1:9:A:ILE:HG13	6	0.67
(4,29)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	8	0.66
(4,29)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	8	0.66
(4,29)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	8	0.66
(4,15)	1:17:A:PRO:HA	1:17:A:PRO:HD3	9	0.66
(3,382)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	2	0.66
(3,285)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.66
(3,285)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.66
(2,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	2	0.66
(2,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	8	0.66
(2,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	8	0.66
(2,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	8	0.66
(2,304)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.66
(2,304)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,201)	1:17:A:PRO:HA	1:17:A:PRO:HD3	9	0.66
(1,441)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	1	0.66
(1,441)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	1	0.66
(1,441)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	1	0.66
(1,434)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	6	0.66
(1,434)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	6	0.66
(1,434)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	6	0.66
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	8	0.66
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	8	0.66
(1,289)	1:15:A:GLY:H	1:16:A:GLY:H	3	0.66
(1,258)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	5	0.66
(1,28)	1:3:A:GLU:HB3	1:4:A:ALA:H	8	0.66
(4,19)	1:11:A:TRP:HA	1:11:A:TRP:HE3	2	0.65
(3,421)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	3	0.65
(3,354)	1:8:A:TYR:HA	1:24:A:PRO:HG2	6	0.65
(2,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	3	0.65
(2,379)	1:8:A:TYR:HA	1:24:A:PRO:HG2	6	0.65
(2,303)	1:11:A:TRP:HA	1:11:A:TRP:HE3	2	0.65
(1,362)	1:14:A:GLN:HE22	1:21:A:ARG:HG2	1	0.65
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	1	0.65
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	1	0.65
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	1	0.65
(1,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	3	0.65
(1,258)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	3	0.65
(1,235)	1:23:A:PRO:HA	1:23:A:PRO:HB3	6	0.65
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	9	0.65
(1,176)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	9	0.65
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	9	0.65
(1,176)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	9	0.65
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG2	7	0.65
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG3	7	0.65
(1,102)	1:9:A:ILE:HA	1:9:A:ILE:HG12	7	0.65
(1,28)	1:3:A:GLU:HB3	1:4:A:ALA:H	9	0.65
(4,19)	1:11:A:TRP:HA	1:11:A:TRP:HE3	5	0.64
(4,15)	1:17:A:PRO:HA	1:17:A:PRO:HD3	10	0.64
(3,423)	1:7:A:LEU:HA	1:10:A:GLN:HB2	8	0.64
(3,173)	1:14:A:GLN:H	1:14:A:GLN:HB2	5	0.64
(2,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	8	0.64
(2,303)	1:11:A:TRP:HA	1:11:A:TRP:HE3	5	0.64
(2,201)	1:17:A:PRO:HA	1:17:A:PRO:HD3	10	0.64
(2,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	5	0.64
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	8	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	8	0.64
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	8	0.64
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	8	0.64
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	8	0.64
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	8	0.64
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	8	0.64
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	8	0.64
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	8	0.64
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	8	0.64
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	8	0.64
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	8	0.64
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG11	8	0.64
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG12	8	0.64
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG13	8	0.64
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG21	8	0.64
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG22	8	0.64
(1,466)	1:2:A:GLU:HA	1:5:A:VAL:HG23	8	0.64
(1,430)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	10	0.64
(1,430)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	10	0.64
(1,430)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	10	0.64
(1,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	8	0.64
(1,408)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	7	0.64
(1,347)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	1	0.64
(1,347)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	5	0.64
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	3	0.64
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	3	0.64
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	3	0.64
(1,305)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	6	0.64
(1,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	1	0.64
(1,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	4	0.64
(1,258)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	1	0.64
(1,258)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	2	0.64
(1,258)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	4	0.64
(1,258)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	9	0.64
(1,235)	1:23:A:PRO:HA	1:23:A:PRO:HB3	1	0.64
(1,235)	1:23:A:PRO:HA	1:23:A:PRO:HB3	2	0.64
(1,235)	1:23:A:PRO:HA	1:23:A:PRO:HB3	4	0.64
(1,235)	1:23:A:PRO:HA	1:23:A:PRO:HB3	9	0.64
(1,235)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.64
(1,52)	1:6:A:ARG:HA	1:6:A:ARG:HG2	3	0.64
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	3	0.63
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	3	0.63
(4,15)	1:17:A:PRO:HA	1:17:A:PRO:HD3	1	0.63
(3,363)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	3	0.63
(3,173)	1:14:A:GLN:H	1:14:A:GLN:HB2	2	0.63
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	8	0.63
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	8	0.63
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	3	0.63
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	3	0.63
(2,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	3	0.63
(2,389)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	3	0.63
(2,201)	1:17:A:PRO:HA	1:17:A:PRO:HD3	1	0.63
(2,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	2	0.63
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	8	0.63
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	8	0.63
(1,341)	1:21:A:ARG:H	1:21:A:ARG:HG2	8	0.63
(1,326)	1:11:A:TRP:HB3	1:12:A:LEU:H	7	0.63
(1,324)	1:10:A:GLN:HE21	1:11:A:TRP:HA	8	0.63
(1,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	8	0.63
(1,258)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.63
(1,235)	1:23:A:PRO:HA	1:23:A:PRO:HB3	3	0.63
(1,235)	1:23:A:PRO:HA	1:23:A:PRO:HB3	5	0.63
(1,235)	1:23:A:PRO:HA	1:23:A:PRO:HB3	7	0.63
(1,235)	1:23:A:PRO:HA	1:23:A:PRO:HB3	8	0.63
(1,194)	1:18:A:SER:H	1:18:A:SER:HB2	10	0.63
(1,194)	1:18:A:SER:H	1:18:A:SER:HB3	10	0.63
(1,102)	1:9:A:ILE:HA	1:9:A:ILE:HG12	8	0.63
(1,102)	1:9:A:ILE:HA	1:9:A:ILE:HG12	9	0.63
(1,102)	1:9:A:ILE:HA	1:9:A:ILE:HG12	10	0.63
(1,54)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	7	0.63
(1,50)	1:6:A:ARG:HA	1:6:A:ARG:HB2	1	0.63
(1,50)	1:6:A:ARG:HA	1:6:A:ARG:HB2	8	0.63
(1,50)	1:6:A:ARG:HA	1:6:A:ARG:HB2	9	0.63
(1,32)	1:3:A:GLU:H	1:4:A:ALA:H	3	0.63
(1,28)	1:3:A:GLU:HB3	1:4:A:ALA:H	4	0.63
(4,29)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	10	0.62
(4,29)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	10	0.62
(4,29)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	10	0.62
(4,15)	1:17:A:PRO:HA	1:17:A:PRO:HD3	4	0.62
(4,15)	1:17:A:PRO:HA	1:17:A:PRO:HD3	8	0.62
(3,364)	1:9:A:ILE:HA	1:12:A:LEU:HB3	6	0.62
(3,264)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	8	0.62
(3,173)	1:14:A:GLN:H	1:14:A:GLN:HB2	4	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,173)	1:14:A:GLN:H	1:14:A:GLN:HB2	6	0.62
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	6	0.62
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	6	0.62
(2,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	10	0.62
(2,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	10	0.62
(2,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	10	0.62
(2,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	6	0.62
(2,281)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	8	0.62
(2,201)	1:17:A:PRO:HA	1:17:A:PRO:HD3	4	0.62
(2,201)	1:17:A:PRO:HA	1:17:A:PRO:HD3	8	0.62
(2,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	4	0.62
(2,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	6	0.62
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	6	0.62
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	6	0.62
(1,430)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	9	0.62
(1,430)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	9	0.62
(1,430)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	9	0.62
(1,305)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	1	0.62
(1,305)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	3	0.62
(1,305)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	7	0.62
(1,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	2	0.62
(1,282)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	10	0.62
(1,187)	1:14:A:GLN:H	1:14:A:GLN:HG2	2	0.62
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	3	0.62
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	3	0.62
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	3	0.62
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	3	0.62
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	5	0.62
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	5	0.62
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	5	0.62
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	5	0.62
(1,154)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	2	0.62
(1,154)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	9	0.62
(1,102)	1:9:A:ILE:HA	1:9:A:ILE:HG12	2	0.62
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD11	8	0.62
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD12	8	0.62
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD13	8	0.62
(1,50)	1:6:A:ARG:HA	1:6:A:ARG:HB2	2	0.62
(1,50)	1:6:A:ARG:HA	1:6:A:ARG:HB2	4	0.62
(1,12)	1:18:A:SER:H	1:18:A:SER:HA	4	0.62
(1,12)	1:18:A:SER:H	1:18:A:SER:HA	6	0.62
(1,12)	1:18:A:SER:H	1:18:A:SER:HA	7	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,421)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	8	0.61
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	2	0.61
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	2	0.61
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	2	0.61
(3,264)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	5	0.61
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	1	0.61
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	1	0.61
(2,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	8	0.61
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	2	0.61
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	2	0.61
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	2	0.61
(2,281)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	5	0.61
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	1	0.61
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	1	0.61
(1,341)	1:21:A:ARG:H	1:21:A:ARG:HG2	3	0.61
(1,305)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	4	0.61
(1,305)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	9	0.61
(1,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	0.61
(1,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.61
(1,187)	1:14:A:GLN:H	1:14:A:GLN:HG2	6	0.61
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	2	0.61
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	2	0.61
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	2	0.61
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	2	0.61
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	4	0.61
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	4	0.61
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	4	0.61
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	4	0.61
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	6	0.61
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	6	0.61
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	6	0.61
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	6	0.61
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	0.61
(1,173)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	10	0.61
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	10	0.61
(1,173)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	10	0.61
(1,154)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	1	0.61
(1,154)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	3	0.61
(1,154)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	4	0.61
(1,154)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	5	0.61
(1,154)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	6	0.61
(1,154)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	7	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	8	0.61
(1,154)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.61
(1,102)	1:9:A:ILE:HA	1:9:A:ILE:HG12	4	0.61
(1,102)	1:9:A:ILE:HA	1:9:A:ILE:HG12	5	0.61
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD11	7	0.61
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD12	7	0.61
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HD13	7	0.61
(1,73)	1:6:A:ARG:HD2	1:7:A:LEU:H	10	0.61
(1,9)	1:25:A:SER:H	1:25:A:SER:HA	8	0.61
(4,41)	1:13:A:LYS:H	1:14:A:GLN:HA	4	0.6
(4,21)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.6
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	3	0.6
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	3	0.6
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	3	0.6
(3,363)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	1	0.6
(3,363)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	4	0.6
(3,176)	1:14:A:GLN:HA	1:14:A:GLN:HG2	3	0.6
(3,173)	1:14:A:GLN:H	1:14:A:GLN:HB2	3	0.6
(3,173)	1:14:A:GLN:H	1:14:A:GLN:HB2	9	0.6
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	2	0.6
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	2	0.6
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	4	0.6
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	4	0.6
(2,472)	1:13:A:LYS:H	1:14:A:GLN:HA	4	0.6
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	3	0.6
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	3	0.6
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	3	0.6
(2,389)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	1	0.6
(2,389)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	4	0.6
(2,325)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.6
(2,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	3	0.6
(2,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	3	0.6
(2,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	9	0.6
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	2	0.6
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	2	0.6
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	4	0.6
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	4	0.6
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	8	0.6
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	8	0.6
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	8	0.6
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	8	0.6
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	8	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	8	0.6
(1,388)	1:5:A:VAL:HA	1:8:A:TYR:HB3	2	0.6
(1,385)	1:7:A:LEU:HD11	1:8:A:TYR:HA	8	0.6
(1,385)	1:7:A:LEU:HD12	1:8:A:TYR:HA	8	0.6
(1,385)	1:7:A:LEU:HD13	1:8:A:TYR:HA	8	0.6
(1,305)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	8	0.6
(1,194)	1:18:A:SER:H	1:18:A:SER:HB2	8	0.6
(1,194)	1:18:A:SER:H	1:18:A:SER:HB3	8	0.6
(1,151)	1:15:A:GLY:HA3	1:16:A:GLY:H	9	0.6
(1,72)	1:6:A:ARG:HD3	1:7:A:LEU:H	1	0.6
(1,69)	1:6:A:ARG:H	1:6:A:ARG:HB3	1	0.6
(1,69)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.6
(1,56)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	7	0.6
(4,19)	1:11:A:TRP:HA	1:11:A:TRP:HE3	4	0.59
(4,19)	1:11:A:TRP:HA	1:11:A:TRP:HE3	9	0.59
(4,19)	1:11:A:TRP:HA	1:11:A:TRP:HE3	10	0.59
(4,15)	1:17:A:PRO:HA	1:17:A:PRO:HD3	3	0.59
(2,303)	1:11:A:TRP:HA	1:11:A:TRP:HE3	4	0.59
(2,303)	1:11:A:TRP:HA	1:11:A:TRP:HE3	9	0.59
(2,303)	1:11:A:TRP:HA	1:11:A:TRP:HE3	10	0.59
(2,201)	1:17:A:PRO:HA	1:17:A:PRO:HD3	3	0.59
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB1	7	0.59
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB2	7	0.59
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB3	7	0.59
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB1	7	0.59
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB2	7	0.59
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB3	7	0.59
(1,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	1	0.59
(1,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	1	0.59
(1,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	7	0.59
(1,409)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	4	0.59
(1,408)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	3	0.59
(1,388)	1:5:A:VAL:HA	1:8:A:TYR:HB3	5	0.59
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	5	0.59
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	5	0.59
(1,270)	1:24:A:PRO:HA	1:24:A:PRO:HG3	3	0.59
(1,256)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	3	0.59
(1,254)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	6	0.59
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	1	0.59
(1,194)	1:18:A:SER:H	1:18:A:SER:HB2	2	0.59
(1,194)	1:18:A:SER:H	1:18:A:SER:HB3	2	0.59
(1,102)	1:9:A:ILE:HA	1:9:A:ILE:HG12	1	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	5	0.59
(1,34)	1:5:A:VAL:HA	1:5:A:VAL:HB	5	0.59
(4,19)	1:11:A:TRP:HA	1:11:A:TRP:HE3	1	0.58
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HG3	10	0.58
(2,303)	1:11:A:TRP:HA	1:11:A:TRP:HE3	1	0.58
(2,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	10	0.58
(1,441)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	4	0.58
(1,441)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	4	0.58
(1,441)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	4	0.58
(1,430)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	3	0.58
(1,430)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	3	0.58
(1,430)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	3	0.58
(1,409)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	1	0.58
(1,408)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	8	0.58
(1,399)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	1	0.58
(1,399)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	1	0.58
(1,399)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	1	0.58
(1,399)	1:5:A:VAL:HG21	1:8:A:TYR:HB3	1	0.58
(1,399)	1:5:A:VAL:HG22	1:8:A:TYR:HB3	1	0.58
(1,399)	1:5:A:VAL:HG23	1:8:A:TYR:HB3	1	0.58
(1,370)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	3	0.58
(1,370)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	3	0.58
(1,370)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	3	0.58
(1,370)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	3	0.58
(1,370)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	3	0.58
(1,370)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	3	0.58
(1,370)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	3	0.58
(1,370)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	3	0.58
(1,370)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	3	0.58
(1,370)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	3	0.58
(1,370)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	3	0.58
(1,370)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	3	0.58
(1,305)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	0.58
(1,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	0.58
(1,209)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	10	0.58
(1,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	1	0.58
(1,186)	1:14:A:GLN:H	1:14:A:GLN:HB3	1	0.58
(1,158)	1:12:A:LEU:HA	1:12:A:LEU:HB3	1	0.58
(1,158)	1:12:A:LEU:HA	1:12:A:LEU:HB3	2	0.58
(1,158)	1:12:A:LEU:HA	1:12:A:LEU:HB3	4	0.58
(1,158)	1:12:A:LEU:HA	1:12:A:LEU:HB3	9	0.58
(1,155)	1:12:A:LEU:HA	1:16:A:GLY:H	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:6:A:ARG:H	1:6:A:ARG:HB3	2	0.58
(1,34)	1:5:A:VAL:HA	1:5:A:VAL:HB	2	0.58
(1,34)	1:5:A:VAL:HA	1:5:A:VAL:HB	3	0.58
(1,34)	1:5:A:VAL:HA	1:5:A:VAL:HB	4	0.58
(1,34)	1:5:A:VAL:HA	1:5:A:VAL:HB	6	0.58
(4,15)	1:17:A:PRO:HA	1:17:A:PRO:HD3	5	0.57
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HG3	9	0.57
(3,394)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	7	0.57
(3,382)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	4	0.57
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD11	5	0.57
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD12	5	0.57
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD13	5	0.57
(2,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	7	0.57
(2,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	4	0.57
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD11	5	0.57
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD12	5	0.57
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD13	5	0.57
(2,201)	1:17:A:PRO:HA	1:17:A:PRO:HD3	5	0.57
(2,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	9	0.57
(1,478)	1:1:A:GLU:HA	1:1:A:GLU:HG2	10	0.57
(1,478)	1:1:A:GLU:HA	1:1:A:GLU:HG3	10	0.57
(1,305)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	2	0.57
(1,305)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	5	0.57
(1,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	0.57
(1,218)	1:22:A:PRO:HA	1:22:A:PRO:HB3	2	0.57
(1,218)	1:22:A:PRO:HA	1:22:A:PRO:HB3	3	0.57
(1,218)	1:22:A:PRO:HA	1:22:A:PRO:HB3	6	0.57
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	3	0.57
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	3	0.57
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	3	0.57
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	3	0.57
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	5	0.57
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	5	0.57
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	5	0.57
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	5	0.57
(1,158)	1:12:A:LEU:HA	1:12:A:LEU:HB3	5	0.57
(1,34)	1:5:A:VAL:HA	1:5:A:VAL:HB	9	0.57
(1,34)	1:5:A:VAL:HA	1:5:A:VAL:HB	10	0.57
(1,28)	1:3:A:GLU:HB3	1:4:A:ALA:H	6	0.57
(1,12)	1:18:A:SER:H	1:18:A:SER:HA	1	0.57
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	6	0.56
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	6	0.56
(3,382)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	8	0.56
(3,173)	1:14:A:GLN:H	1:14:A:GLN:HB2	10	0.56
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	6	0.56
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	6	0.56
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	6	0.56
(2,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	8	0.56
(2,186)	1:14:A:GLN:H	1:14:A:GLN:HB2	10	0.56
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	4	0.56
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	4	0.56
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	4	0.56
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	4	0.56
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	4	0.56
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	4	0.56
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	4	0.56
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	4	0.56
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	4	0.56
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	4	0.56
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	4	0.56
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	4	0.56
(1,441)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	2	0.56
(1,441)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	2	0.56
(1,441)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	2	0.56
(1,409)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	2	0.56
(1,388)	1:5:A:VAL:HA	1:8:A:TYR:HB3	4	0.56
(1,341)	1:21:A:ARG:H	1:21:A:ARG:HG2	6	0.56
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	3	0.56
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	3	0.56
(1,218)	1:22:A:PRO:HA	1:22:A:PRO:HB3	7	0.56
(1,209)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	5	0.56
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	1	0.56
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	1	0.56
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	1	0.56
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	1	0.56
(1,69)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.56
(1,50)	1:6:A:ARG:HA	1:6:A:ARG:HB2	10	0.56
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG2	5	0.56
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG3	5	0.56
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG2	10	0.56
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG3	10	0.56
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	8	0.55
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,411)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	8	0.55
(3,381)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	2	0.55
(3,364)	1:9:A:ILE:HA	1:12:A:LEU:HB3	3	0.55
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	9	0.55
(3,165)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	9	0.55
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	8	0.55
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	8	0.55
(2,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	8	0.55
(2,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	2	0.55
(2,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	3	0.55
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	9	0.55
(2,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	9	0.55
(1,478)	1:1:A:GLU:HA	1:1:A:GLU:HG2	9	0.55
(1,478)	1:1:A:GLU:HA	1:1:A:GLU:HG3	9	0.55
(1,359)	1:8:A:TYR:HD1	1:12:A:LEU:HG	2	0.55
(1,359)	1:8:A:TYR:HD2	1:12:A:LEU:HG	2	0.55
(1,359)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	2	0.55
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	8	0.55
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	8	0.55
(1,308)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	8	0.55
(1,258)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	6	0.55
(1,243)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	6	0.55
(1,243)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.55
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	3	0.55
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	3	0.55
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	2	0.55
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	2	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	2	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	2	0.55
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	4	0.55
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	4	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	4	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	4	0.55
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	6	0.55
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	6	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	6	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	6	0.55
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	8	0.55
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	8	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	8	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	8	0.55
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	9	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	9	0.55
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	9	0.55
(1,158)	1:12:A:LEU:HA	1:12:A:LEU:HB3	6	0.55
(1,73)	1:6:A:ARG:HD2	1:7:A:LEU:H	3	0.55
(1,56)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	6	0.55
(1,34)	1:5:A:VAL:HA	1:5:A:VAL:HB	7	0.55
(1,34)	1:5:A:VAL:HA	1:5:A:VAL:HB	8	0.55
(1,26)	1:3:A:GLU:HG2	1:4:A:ALA:H	3	0.55
(1,26)	1:3:A:GLU:HG3	1:4:A:ALA:H	3	0.55
(1,12)	1:18:A:SER:H	1:18:A:SER:HA	2	0.55
(1,12)	1:18:A:SER:H	1:18:A:SER:HA	3	0.55
(1,12)	1:18:A:SER:H	1:18:A:SER:HA	8	0.55
(3,381)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	5	0.54
(3,360)	1:15:A:GLY:HA3	1:18:A:SER:HB3	8	0.54
(3,286)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	6	0.54
(3,106)	1:9:A:ILE:H	1:9:A:ILE:HG12	3	0.54
(2,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	5	0.54
(2,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	8	0.54
(2,306)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	6	0.54
(2,116)	1:9:A:ILE:H	1:9:A:ILE:HG12	3	0.54
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB2	6	0.54
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB3	6	0.54
(1,444)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	6	0.54
(1,444)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	6	0.54
(1,444)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	6	0.54
(1,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	6	0.54
(1,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	6	0.54
(1,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	6	0.54
(1,431)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	10	0.54
(1,431)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	10	0.54
(1,431)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	10	0.54
(1,359)	1:8:A:TYR:HD1	1:12:A:LEU:HG	4	0.54
(1,359)	1:8:A:TYR:HD2	1:12:A:LEU:HG	4	0.54
(1,359)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	4	0.54
(1,319)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	4	0.54
(1,319)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	10	0.54
(1,314)	1:8:A:TYR:HD1	1:9:A:ILE:H	3	0.54
(1,314)	1:8:A:TYR:HD2	1:9:A:ILE:H	3	0.54
(1,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.54
(1,282)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	3	0.54
(1,270)	1:24:A:PRO:HA	1:24:A:PRO:HG3	1	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	1	0.54
(1,243)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	2	0.54
(1,243)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	3	0.54
(1,243)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	4	0.54
(1,243)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	5	0.54
(1,243)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	7	0.54
(1,243)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	8	0.54
(1,243)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	9	0.54
(1,218)	1:22:A:PRO:HA	1:22:A:PRO:HB3	4	0.54
(1,218)	1:22:A:PRO:HA	1:22:A:PRO:HB3	8	0.54
(1,209)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	8	0.54
(1,158)	1:12:A:LEU:HA	1:12:A:LEU:HB3	7	0.54
(1,158)	1:12:A:LEU:HA	1:12:A:LEU:HB3	10	0.54
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG2	4	0.54
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG3	4	0.54
(1,12)	1:18:A:SER:H	1:18:A:SER:HA	10	0.54
(3,394)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	3	0.53
(3,381)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	4	0.53
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	4	0.53
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	4	0.53
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	4	0.53
(3,106)	1:9:A:ILE:H	1:9:A:ILE:HG12	6	0.53
(2,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	3	0.53
(2,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	4	0.53
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	4	0.53
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	4	0.53
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	4	0.53
(2,116)	1:9:A:ILE:H	1:9:A:ILE:HG12	6	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB2	1	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB3	1	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB2	2	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB3	2	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB2	3	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB3	3	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB2	4	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB3	4	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB2	7	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB3	7	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB2	8	0.53
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB3	8	0.53
(1,444)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	4	0.53
(1,444)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,444)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	4	0.53
(1,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	4	0.53
(1,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	4	0.53
(1,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	4	0.53
(1,444)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	5	0.53
(1,444)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	5	0.53
(1,444)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	5	0.53
(1,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	5	0.53
(1,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	5	0.53
(1,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	5	0.53
(1,376)	1:8:A:TYR:HA	1:24:A:PRO:HD3	6	0.53
(1,359)	1:8:A:TYR:HD1	1:12:A:LEU:HG	1	0.53
(1,359)	1:8:A:TYR:HD2	1:12:A:LEU:HG	1	0.53
(1,359)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	1	0.53
(1,347)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	6	0.53
(1,343)	1:10:A:GLN:HE21	1:14:A:GLN:HG3	7	0.53
(1,338)	1:21:A:ARG:H	1:21:A:ARG:HB2	5	0.53
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	7	0.53
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	7	0.53
(1,319)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	1	0.53
(1,319)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	6	0.53
(1,299)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	9	0.53
(1,256)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	9	0.53
(1,240)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	1	0.53
(1,240)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	3	0.53
(1,240)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	5	0.53
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	1	0.53
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	1	0.53
(1,218)	1:22:A:PRO:HA	1:22:A:PRO:HB3	1	0.53
(1,218)	1:22:A:PRO:HA	1:22:A:PRO:HB3	5	0.53
(1,218)	1:22:A:PRO:HA	1:22:A:PRO:HB3	9	0.53
(1,59)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	6	0.53
(1,56)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	5	0.53
(1,50)	1:6:A:ARG:HA	1:6:A:ARG:HB2	3	0.53
(3,394)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	6	0.52
(3,381)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	1	0.52
(3,381)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	9	0.52
(3,106)	1:9:A:ILE:H	1:9:A:ILE:HG12	9	0.52
(2,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	6	0.52
(2,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	1	0.52
(2,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	9	0.52
(2,116)	1:9:A:ILE:H	1:9:A:ILE:HG12	9	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	7	0.52
(1,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	7	0.52
(1,444)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	2	0.52
(1,444)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	2	0.52
(1,444)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	2	0.52
(1,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	2	0.52
(1,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	2	0.52
(1,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	2	0.52
(1,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	3	0.52
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	4	0.52
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	4	0.52
(1,327)	1:8:A:TYR:HB3	1:9:A:ILE:H	6	0.52
(1,319)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	2	0.52
(1,314)	1:8:A:TYR:HD1	1:9:A:ILE:H	7	0.52
(1,314)	1:8:A:TYR:HD2	1:9:A:ILE:H	7	0.52
(1,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	0.52
(1,270)	1:24:A:PRO:HA	1:24:A:PRO:HG3	2	0.52
(1,270)	1:24:A:PRO:HA	1:24:A:PRO:HG3	9	0.52
(1,240)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	2	0.52
(1,240)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	4	0.52
(1,240)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	6	0.52
(1,240)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	7	0.52
(1,240)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	8	0.52
(1,240)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	9	0.52
(1,240)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	10	0.52
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	4	0.52
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	4	0.52
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	5	0.52
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	5	0.52
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	7	0.52
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	7	0.52
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	9	0.52
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	9	0.52
(1,218)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.52
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG2	5	0.52
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG3	5	0.52
(1,155)	1:12:A:LEU:HA	1:16:A:GLY:H	4	0.52
(1,73)	1:6:A:ARG:HD2	1:7:A:LEU:H	2	0.52
(1,12)	1:18:A:SER:H	1:18:A:SER:HA	5	0.52
(1,12)	1:18:A:SER:H	1:18:A:SER:HA	9	0.52
(1,10)	1:15:A:GLY:H	1:15:A:GLY:HA2	6	0.52
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.51
(4,15)	1:17:A:PRO:HA	1:17:A:PRO:HD3	7	0.51
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD11	7	0.51
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD12	7	0.51
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD13	7	0.51
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	8	0.51
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	8	0.51
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	8	0.51
(3,175)	1:14:A:GLN:H	1:14:A:GLN:HG3	1	0.51
(3,168)	1:13:A:LYS:H	1:13:A:LYS:HB3	9	0.51
(3,106)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.51
(3,106)	1:9:A:ILE:H	1:9:A:ILE:HG12	2	0.51
(3,106)	1:9:A:ILE:H	1:9:A:ILE:HG12	5	0.51
(3,106)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.51
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD11	7	0.51
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD12	7	0.51
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD13	7	0.51
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	8	0.51
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	8	0.51
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	8	0.51
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.51
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.51
(2,201)	1:17:A:PRO:HA	1:17:A:PRO:HD3	7	0.51
(2,188)	1:14:A:GLN:H	1:14:A:GLN:HG3	1	0.51
(2,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	9	0.51
(2,116)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.51
(2,116)	1:9:A:ILE:H	1:9:A:ILE:HG12	2	0.51
(2,116)	1:9:A:ILE:H	1:9:A:ILE:HG12	5	0.51
(2,116)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.51
(1,420)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	1	0.51
(1,420)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	1	0.51
(1,420)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	7	0.51
(1,420)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	7	0.51
(1,270)	1:24:A:PRO:HA	1:24:A:PRO:HG3	4	0.51
(1,249)	1:25:A:SER:H	1:25:A:SER:HB2	9	0.51
(1,249)	1:25:A:SER:H	1:25:A:SER:HB3	9	0.51
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	10	0.51
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	10	0.51
(1,209)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	3	0.51
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	7	0.51
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	7	0.51
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	7	0.51
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	0.51
(1,179)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	0.51
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	10	0.51
(1,179)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	10	0.51
(1,158)	1:12:A:LEU:HA	1:12:A:LEU:HB3	3	0.51
(1,69)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.51
(1,28)	1:3:A:GLU:HB3	1:4:A:ALA:H	10	0.51
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG2	7	0.51
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG3	7	0.51
(1,10)	1:15:A:GLY:H	1:15:A:GLY:HA2	4	0.51
(1,10)	1:15:A:GLY:H	1:15:A:GLY:HA2	8	0.51
(3,360)	1:15:A:GLY:HA3	1:18:A:SER:HB3	9	0.5
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	1	0.5
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	4	0.5
(3,182)	1:19:A:SER:HA	1:19:A:SER:HB3	9	0.5
(3,106)	1:9:A:ILE:H	1:9:A:ILE:HG12	4	0.5
(2,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	9	0.5
(2,333)	1:12:A:LEU:HB3	1:13:A:LYS:H	1	0.5
(2,333)	1:12:A:LEU:HB3	1:13:A:LYS:H	4	0.5
(2,196)	1:19:A:SER:HA	1:19:A:SER:HB3	9	0.5
(2,116)	1:9:A:ILE:H	1:9:A:ILE:HG12	4	0.5
(1,430)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	5	0.5
(1,430)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	5	0.5
(1,430)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	5	0.5
(1,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.5
(1,385)	1:7:A:LEU:HD11	1:8:A:TYR:HA	2	0.5
(1,385)	1:7:A:LEU:HD12	1:8:A:TYR:HA	2	0.5
(1,385)	1:7:A:LEU:HD13	1:8:A:TYR:HA	2	0.5
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	2	0.5
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	2	0.5
(1,256)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	1	0.5
(1,256)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	4	0.5
(1,256)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	5	0.5
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	2	0.5
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	2	0.5
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	8	0.5
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	8	0.5
(1,209)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	7	0.5
(1,158)	1:12:A:LEU:HA	1:12:A:LEU:HB3	8	0.5
(1,107)	1:9:A:ILE:HB	1:9:A:ILE:HG13	6	0.5
(1,73)	1:6:A:ARG:HD2	1:7:A:LEU:H	8	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG2	8	0.5
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG3	8	0.5
(1,10)	1:15:A:GLY:H	1:15:A:GLY:HA2	1	0.5
(4,21)	1:8:A:TYR:HB2	1:9:A:ILE:H	3	0.49
(4,21)	1:8:A:TYR:HB2	1:9:A:ILE:H	5	0.49
(4,19)	1:11:A:TRP:HA	1:11:A:TRP:HE3	7	0.49
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.49
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.49
(3,363)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	5	0.49
(3,363)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.49
(3,175)	1:14:A:GLN:H	1:14:A:GLN:HG3	7	0.49
(2,389)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	5	0.49
(2,389)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.49
(2,325)	1:8:A:TYR:HB2	1:9:A:ILE:H	3	0.49
(2,325)	1:8:A:TYR:HB2	1:9:A:ILE:H	5	0.49
(2,303)	1:11:A:TRP:HA	1:11:A:TRP:HE3	7	0.49
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.49
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.49
(2,188)	1:14:A:GLN:H	1:14:A:GLN:HG3	7	0.49
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB1	8	0.49
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB2	8	0.49
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB3	8	0.49
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB1	8	0.49
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB2	8	0.49
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB3	8	0.49
(1,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	4	0.49
(1,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	4	0.49
(1,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	5	0.49
(1,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	5	0.49
(1,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	1	0.49
(1,367)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	4	0.49
(1,367)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	4	0.49
(1,356)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	9	0.49
(1,341)	1:21:A:ARG:H	1:21:A:ARG:HG2	1	0.49
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	9	0.49
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	9	0.49
(1,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	0.49
(1,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	0.49
(1,288)	1:13:A:LYS:H	1:14:A:GLN:H	1	0.49
(1,282)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	4	0.49
(1,261)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	1	0.49
(1,261)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	4	0.49
(1,25)	1:3:A:GLU:HG2	1:4:A:ALA:HA	3	0.49
(1,25)	1:3:A:GLU:HG3	1:4:A:ALA:HA	3	0.49
(1,10)	1:15:A:GLY:H	1:15:A:GLY:HA2	2	0.49
(4,41)	1:13:A:LYS:H	1:14:A:GLN:HA	3	0.48
(4,41)	1:13:A:LYS:H	1:14:A:GLN:HA	6	0.48
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.48
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.48
(3,363)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	2	0.48
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	2	0.48
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	5	0.48
(2,472)	1:13:A:LYS:H	1:14:A:GLN:HA	3	0.48
(2,472)	1:13:A:LYS:H	1:14:A:GLN:HA	6	0.48
(2,389)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	2	0.48
(2,333)	1:12:A:LEU:HB3	1:13:A:LYS:H	2	0.48
(2,333)	1:12:A:LEU:HB3	1:13:A:LYS:H	5	0.48
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.48
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.48
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	10	0.48
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB3	10	0.48
(1,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	0.48
(1,388)	1:5:A:VAL:HA	1:8:A:TYR:HB3	6	0.48
(1,388)	1:5:A:VAL:HA	1:8:A:TYR:HB3	7	0.48
(1,388)	1:5:A:VAL:HA	1:8:A:TYR:HB3	9	0.48
(1,385)	1:7:A:LEU:HD11	1:8:A:TYR:HA	10	0.48
(1,385)	1:7:A:LEU:HD12	1:8:A:TYR:HA	10	0.48
(1,385)	1:7:A:LEU:HD13	1:8:A:TYR:HA	10	0.48
(1,370)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	10	0.48
(1,370)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	10	0.48
(1,370)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	10	0.48
(1,370)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	10	0.48
(1,370)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	10	0.48
(1,370)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	10	0.48
(1,370)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	10	0.48
(1,370)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	10	0.48
(1,370)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	10	0.48
(1,370)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	10	0.48
(1,370)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	10	0.48
(1,370)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	10	0.48
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	1	0.48
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	1	0.48
(1,284)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	9	0.48
(1,282)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	7	0.48
(1,278)	1:21:A:ARG:HA	1:21:A:ARG:HB3	7	0.48
(1,256)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	2	0.48
(1,254)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.48
(1,209)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	6	0.48
(1,209)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	9	0.48
(1,107)	1:9:A:ILE:HB	1:9:A:ILE:HG13	2	0.48
(1,107)	1:9:A:ILE:HB	1:9:A:ILE:HG13	3	0.48
(1,107)	1:9:A:ILE:HB	1:9:A:ILE:HG13	10	0.48
(1,73)	1:6:A:ARG:HD2	1:7:A:LEU:H	1	0.48
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG2	6	0.48
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG3	6	0.48
(1,10)	1:15:A:GLY:H	1:15:A:GLY:HA2	10	0.48
(4,41)	1:13:A:LYS:H	1:14:A:GLN:HA	2	0.47
(4,41)	1:13:A:LYS:H	1:14:A:GLN:HA	5	0.47
(4,19)	1:11:A:TRP:HA	1:11:A:TRP:HE3	6	0.47
(3,364)	1:9:A:ILE:HA	1:12:A:LEU:HB3	8	0.47
(3,327)	1:24:A:PRO:HB3	1:25:A:SER:H	6	0.47
(3,106)	1:9:A:ILE:H	1:9:A:ILE:HG12	8	0.47
(3,44)	1:5:A:VAL:HB	1:6:A:ARG:H	5	0.47
(3,44)	1:5:A:VAL:HB	1:6:A:ARG:H	6	0.47
(2,472)	1:13:A:LYS:H	1:14:A:GLN:HA	2	0.47
(2,472)	1:13:A:LYS:H	1:14:A:GLN:HA	5	0.47
(2,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	8	0.47
(2,349)	1:24:A:PRO:HB3	1:25:A:SER:H	6	0.47
(2,303)	1:11:A:TRP:HA	1:11:A:TRP:HE3	6	0.47
(2,116)	1:9:A:ILE:H	1:9:A:ILE:HG12	8	0.47
(2,46)	1:5:A:VAL:HB	1:6:A:ARG:H	5	0.47
(2,46)	1:5:A:VAL:HB	1:6:A:ARG:H	6	0.47
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	3	0.47
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	3	0.47
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	3	0.47
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	3	0.47
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	3	0.47
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	3	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	3	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	3	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	3	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	3	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	3	0.47
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	3	0.47
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB3	3	0.47
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	5	0.47
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB3	5	0.47
(1,444)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	3	0.47
(1,444)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	3	0.47
(1,444)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	3	0.47
(1,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	3	0.47
(1,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	3	0.47
(1,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	3	0.47
(1,430)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	2	0.47
(1,430)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	2	0.47
(1,430)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	2	0.47
(1,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	0.47
(1,385)	1:7:A:LEU:HD11	1:8:A:TYR:HA	3	0.47
(1,385)	1:7:A:LEU:HD12	1:8:A:TYR:HA	3	0.47
(1,385)	1:7:A:LEU:HD13	1:8:A:TYR:HA	3	0.47
(1,356)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.47
(1,338)	1:21:A:ARG:H	1:21:A:ARG:HB2	9	0.47
(1,270)	1:24:A:PRO:HA	1:24:A:PRO:HG3	7	0.47
(1,270)	1:24:A:PRO:HA	1:24:A:PRO:HG3	8	0.47
(1,261)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	8	0.47
(1,261)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	9	0.47
(1,209)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	1	0.47
(1,182)	1:13:A:LYS:H	1:13:A:LYS:HD2	8	0.47
(1,182)	1:13:A:LYS:H	1:13:A:LYS:HD3	8	0.47
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG2	3	0.47
(1,175)	1:13:A:LYS:HA	1:13:A:LYS:HG3	3	0.47
(1,107)	1:9:A:ILE:HB	1:9:A:ILE:HG13	4	0.47
(1,107)	1:9:A:ILE:HB	1:9:A:ILE:HG13	5	0.47
(1,107)	1:9:A:ILE:HB	1:9:A:ILE:HG13	9	0.47
(1,67)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	5	0.47
(1,67)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	7	0.47
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG11	3	0.47
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG12	3	0.47
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG13	3	0.47
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG21	3	0.47
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG22	3	0.47
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG23	3	0.47
(1,10)	1:15:A:GLY:H	1:15:A:GLY:HA2	5	0.47
(4,21)	1:8:A:TYR:HB2	1:9:A:ILE:H	2	0.46
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.46
(4,15)	1:17:A:PRO:HA	1:17:A:PRO:HD3	6	0.46
(4,3)	1:6:A:ARG:HA	1:6:A:ARG:HD2	9	0.46
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD11	6	0.46
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD12	6	0.46
(3,374)	1:6:A:ARG:HD3	1:7:A:LEU:HD13	6	0.46
(3,168)	1:13:A:LYS:H	1:13:A:LYS:HB3	6	0.46
(3,106)	1:9:A:ILE:H	1:9:A:ILE:HG12	7	0.46
(3,44)	1:5:A:VAL:HB	1:6:A:ARG:H	4	0.46
(3,44)	1:5:A:VAL:HB	1:6:A:ARG:H	7	0.46
(3,44)	1:5:A:VAL:HB	1:6:A:ARG:H	9	0.46
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD11	6	0.46
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD12	6	0.46
(2,403)	1:6:A:ARG:HD3	1:7:A:LEU:HD13	6	0.46
(2,325)	1:8:A:TYR:HB2	1:9:A:ILE:H	2	0.46
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.46
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.46
(2,201)	1:17:A:PRO:HA	1:17:A:PRO:HD3	6	0.46
(2,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	6	0.46
(2,116)	1:9:A:ILE:H	1:9:A:ILE:HG12	7	0.46
(2,48)	1:6:A:ARG:HA	1:6:A:ARG:HD2	9	0.46
(2,46)	1:5:A:VAL:HB	1:6:A:ARG:H	4	0.46
(2,46)	1:5:A:VAL:HB	1:6:A:ARG:H	7	0.46
(2,46)	1:5:A:VAL:HB	1:6:A:ARG:H	9	0.46
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	9	0.46
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB3	9	0.46
(1,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	10	0.46
(1,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB3	10	0.46
(1,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	10	0.46
(1,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB3	10	0.46
(1,420)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	8	0.46
(1,420)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	8	0.46
(1,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	0.46
(1,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	0.46
(1,385)	1:7:A:LEU:HD11	1:8:A:TYR:HA	7	0.46
(1,385)	1:7:A:LEU:HD12	1:8:A:TYR:HA	7	0.46
(1,385)	1:7:A:LEU:HD13	1:8:A:TYR:HA	7	0.46
(1,381)	1:6:A:ARG:HA	1:9:A:ILE:HB	1	0.46
(1,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	2	0.46
(1,327)	1:8:A:TYR:HB3	1:9:A:ILE:H	8	0.46
(1,314)	1:8:A:TYR:HD1	1:9:A:ILE:H	5	0.46
(1,314)	1:8:A:TYR:HD2	1:9:A:ILE:H	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,289)	1:15:A:GLY:H	1:16:A:GLY:H	7	0.46
(1,284)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	2	0.46
(1,270)	1:24:A:PRO:HA	1:24:A:PRO:HG3	5	0.46
(1,261)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	5	0.46
(1,256)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	7	0.46
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD2	6	0.46
(1,233)	1:23:A:PRO:HB2	1:23:A:PRO:HD3	6	0.46
(1,107)	1:9:A:ILE:HB	1:9:A:ILE:HG13	1	0.46
(1,67)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	6	0.46
(1,59)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	7	0.46
(1,28)	1:3:A:GLU:HB3	1:4:A:ALA:H	7	0.46
(1,10)	1:15:A:GLY:H	1:15:A:GLY:HA2	7	0.46
(4,21)	1:8:A:TYR:HB2	1:9:A:ILE:H	4	0.45
(4,19)	1:11:A:TRP:HA	1:11:A:TRP:HE3	8	0.45
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.45
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.45
(3,44)	1:5:A:VAL:HB	1:6:A:ARG:H	2	0.45
(3,44)	1:5:A:VAL:HB	1:6:A:ARG:H	3	0.45
(2,325)	1:8:A:TYR:HB2	1:9:A:ILE:H	4	0.45
(2,303)	1:11:A:TRP:HA	1:11:A:TRP:HE3	8	0.45
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.45
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.45
(2,46)	1:5:A:VAL:HB	1:6:A:ARG:H	2	0.45
(2,46)	1:5:A:VAL:HB	1:6:A:ARG:H	3	0.45
(1,385)	1:7:A:LEU:HD11	1:8:A:TYR:HA	4	0.45
(1,385)	1:7:A:LEU:HD12	1:8:A:TYR:HA	4	0.45
(1,385)	1:7:A:LEU:HD13	1:8:A:TYR:HA	4	0.45
(1,385)	1:7:A:LEU:HD11	1:8:A:TYR:HA	6	0.45
(1,385)	1:7:A:LEU:HD12	1:8:A:TYR:HA	6	0.45
(1,385)	1:7:A:LEU:HD13	1:8:A:TYR:HA	6	0.45
(1,381)	1:6:A:ARG:HA	1:9:A:ILE:HB	8	0.45
(1,354)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	5	0.45
(1,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	0.45
(1,261)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	7	0.45
(1,209)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	4	0.45
(1,107)	1:9:A:ILE:HB	1:9:A:ILE:HG13	7	0.45
(1,107)	1:9:A:ILE:HB	1:9:A:ILE:HG13	8	0.45
(1,73)	1:6:A:ARG:HD2	1:7:A:LEU:H	4	0.45
(1,52)	1:6:A:ARG:HA	1:6:A:ARG:HG2	10	0.45
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG2	2	0.45
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG3	2	0.45
(4,21)	1:8:A:TYR:HB2	1:9:A:ILE:H	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,21)	1:8:A:TYR:HB2	1:9:A:ILE:H	9	0.44
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.44
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.44
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.44
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.44
(3,381)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	6	0.44
(3,333)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	6	0.44
(3,333)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	6	0.44
(3,319)	1:21:A:ARG:H	1:21:A:ARG:HG2	9	0.44
(3,44)	1:5:A:VAL:HB	1:6:A:ARG:H	10	0.44
(2,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	6	0.44
(2,355)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	6	0.44
(2,355)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	6	0.44
(2,341)	1:21:A:ARG:H	1:21:A:ARG:HG2	9	0.44
(2,325)	1:8:A:TYR:HB2	1:9:A:ILE:H	1	0.44
(2,325)	1:8:A:TYR:HB2	1:9:A:ILE:H	9	0.44
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.44
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.44
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.44
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.44
(2,46)	1:5:A:VAL:HB	1:6:A:ARG:H	10	0.44
(1,465)	1:3:A:GLU:HA	1:6:A:ARG:HB3	5	0.44
(1,441)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	9	0.44
(1,441)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	9	0.44
(1,441)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	9	0.44
(1,385)	1:7:A:LEU:HD11	1:8:A:TYR:HA	9	0.44
(1,385)	1:7:A:LEU:HD12	1:8:A:TYR:HA	9	0.44
(1,385)	1:7:A:LEU:HD13	1:8:A:TYR:HA	9	0.44
(1,319)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	8	0.44
(1,261)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	3	0.44
(1,252)	1:23:A:PRO:HA	1:24:A:PRO:HD3	10	0.44
(1,249)	1:25:A:SER:H	1:25:A:SER:HB2	6	0.44
(1,249)	1:25:A:SER:H	1:25:A:SER:HB3	6	0.44
(1,231)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	1	0.44
(1,231)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	1	0.44
(1,231)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	2	0.44
(1,231)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	2	0.44
(1,231)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	3	0.44
(1,231)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	3	0.44
(1,231)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	4	0.44
(1,231)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	4	0.44
(1,231)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	5	0.44
(1,231)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	6	0.44
(1,231)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	6	0.44
(1,231)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	7	0.44
(1,231)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	7	0.44
(1,231)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	8	0.44
(1,231)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	8	0.44
(1,231)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.44
(1,231)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	10	0.44
(1,213)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	1	0.44
(1,213)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	2	0.44
(1,213)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	3	0.44
(1,213)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	4	0.44
(1,213)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	5	0.44
(1,213)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	6	0.44
(1,213)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	7	0.44
(1,213)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	8	0.44
(1,213)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	9	0.44
(1,213)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.44
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB2	3	0.44
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB3	3	0.44
(1,166)	1:12:A:LEU:HD11	1:12:A:LEU:HG	4	0.44
(1,166)	1:12:A:LEU:HD12	1:12:A:LEU:HG	4	0.44
(1,166)	1:12:A:LEU:HD13	1:12:A:LEU:HG	4	0.44
(1,166)	1:12:A:LEU:HD11	1:12:A:LEU:HG	6	0.44
(1,166)	1:12:A:LEU:HD12	1:12:A:LEU:HG	6	0.44
(1,166)	1:12:A:LEU:HD13	1:12:A:LEU:HG	6	0.44
(1,166)	1:12:A:LEU:HD11	1:12:A:LEU:HG	9	0.44
(1,166)	1:12:A:LEU:HD12	1:12:A:LEU:HG	9	0.44
(1,166)	1:12:A:LEU:HD13	1:12:A:LEU:HG	9	0.44
(1,166)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.44
(1,166)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.44
(1,166)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.44
(1,152)	1:16:A:GLY:H	1:16:A:GLY:HA2	9	0.44
(1,150)	1:15:A:GLY:HA2	1:16:A:GLY:H	10	0.44
(1,28)	1:3:A:GLU:HB3	1:4:A:ALA:H	5	0.44
(4,41)	1:13:A:LYS:H	1:14:A:GLN:HA	1	0.43
(4,31)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	7	0.43
(4,28)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	2	0.43
(4,28)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	2	0.43
(4,28)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	2	0.43
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,472)	1:13:A:LYS:H	1:14:A:GLN:HA	1	0.43
(2,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	7	0.43
(2,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	2	0.43
(2,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	2	0.43
(2,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	2	0.43
(2,333)	1:12:A:LEU:HB3	1:13:A:LYS:H	9	0.43
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	1	0.43
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	1	0.43
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	1	0.43
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	1	0.43
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	1	0.43
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	1	0.43
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	1	0.43
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	1	0.43
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	1	0.43
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	1	0.43
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	1	0.43
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	1	0.43
(1,468)	1:5:A:VAL:HG11	1:6:A:ARG:HA	7	0.43
(1,468)	1:5:A:VAL:HG12	1:6:A:ARG:HA	7	0.43
(1,468)	1:5:A:VAL:HG13	1:6:A:ARG:HA	7	0.43
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:HA	7	0.43
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:HA	7	0.43
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:HA	7	0.43
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	5	0.43
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	5	0.43
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	5	0.43
(1,385)	1:7:A:LEU:HD11	1:8:A:TYR:HA	1	0.43
(1,385)	1:7:A:LEU:HD12	1:8:A:TYR:HA	1	0.43
(1,385)	1:7:A:LEU:HD13	1:8:A:TYR:HA	1	0.43
(1,381)	1:6:A:ARG:HA	1:9:A:ILE:HB	4	0.43
(1,361)	1:14:A:GLN:HE22	1:21:A:ARG:HG3	6	0.43
(1,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	6	0.43
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	6	0.43
(1,328)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	6	0.43
(1,314)	1:8:A:TYR:HD1	1:9:A:ILE:H	2	0.43
(1,314)	1:8:A:TYR:HD2	1:9:A:ILE:H	2	0.43
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	9	0.43
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	9	0.43
(1,288)	1:13:A:LYS:H	1:14:A:GLN:H	2	0.43
(1,282)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	1	0.43
(1,231)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	9	0.43
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD2	1	0.43
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD3	1	0.43
(1,166)	1:12:A:LEU:HD11	1:12:A:LEU:HG	1	0.43
(1,166)	1:12:A:LEU:HD12	1:12:A:LEU:HG	1	0.43
(1,166)	1:12:A:LEU:HD13	1:12:A:LEU:HG	1	0.43
(1,166)	1:12:A:LEU:HD11	1:12:A:LEU:HG	2	0.43
(1,166)	1:12:A:LEU:HD12	1:12:A:LEU:HG	2	0.43
(1,166)	1:12:A:LEU:HD13	1:12:A:LEU:HG	2	0.43
(1,166)	1:12:A:LEU:HD11	1:12:A:LEU:HG	3	0.43
(1,166)	1:12:A:LEU:HD12	1:12:A:LEU:HG	3	0.43
(1,166)	1:12:A:LEU:HD13	1:12:A:LEU:HG	3	0.43
(1,166)	1:12:A:LEU:HD11	1:12:A:LEU:HG	5	0.43
(1,166)	1:12:A:LEU:HD12	1:12:A:LEU:HG	5	0.43
(1,166)	1:12:A:LEU:HD13	1:12:A:LEU:HG	5	0.43
(1,166)	1:12:A:LEU:HD11	1:12:A:LEU:HG	8	0.43
(1,166)	1:12:A:LEU:HD12	1:12:A:LEU:HG	8	0.43
(1,166)	1:12:A:LEU:HD13	1:12:A:LEU:HG	8	0.43
(1,50)	1:6:A:ARG:HA	1:6:A:ARG:HB2	5	0.43
(1,50)	1:6:A:ARG:HA	1:6:A:ARG:HB2	6	0.43
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG11	10	0.43
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG12	10	0.43
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG13	10	0.43
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG21	10	0.43
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG22	10	0.43
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG23	10	0.43
(1,25)	1:3:A:GLU:HG2	1:4:A:ALA:HA	1	0.43
(1,25)	1:3:A:GLU:HG3	1:4:A:ALA:HA	1	0.43
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG2	1	0.43
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG3	1	0.43
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG2	3	0.43
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG3	3	0.43
(1,10)	1:15:A:GLY:H	1:15:A:GLY:HA2	9	0.43
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	9	0.42
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	9	0.42
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	9	0.42
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	9	0.42
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	9	0.42
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	9	0.42
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	9	0.42
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	9	0.42
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	9	0.42
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	9	0.42
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	9	0.42
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	9	0.42
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	9	0.42
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	9	0.42
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	9	0.42
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	9	0.42
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	9	0.42
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.42
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.42
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HG3	4	0.42
(3,44)	1:5:A:VAL:HB	1:6:A:ARG:H	8	0.42
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	9	0.42
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	9	0.42
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	9	0.42
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	9	0.42
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	9	0.42
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	9	0.42
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	9	0.42
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	9	0.42
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	9	0.42
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	9	0.42
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	9	0.42
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	9	0.42
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	9	0.42
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	9	0.42
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	9	0.42
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	9	0.42
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	9	0.42
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	9	0.42
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.42
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.42
(2,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	4	0.42
(2,46)	1:5:A:VAL:HB	1:6:A:ARG:H	8	0.42
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	1	0.42
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB3	1	0.42
(1,460)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	2	0.42
(1,460)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	2	0.42
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	7	0.42
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	7	0.42
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	7	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:13:A:LYS:H	1:14:A:GLN:H	5	0.42
(1,261)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.42
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD2	4	0.42
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD3	4	0.42
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD2	5	0.42
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD3	5	0.42
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD2	8	0.42
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD3	8	0.42
(1,192)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	2	0.42
(1,192)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	3	0.42
(1,192)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	6	0.42
(1,192)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	7	0.42
(1,166)	1:12:A:LEU:HD11	1:12:A:LEU:HG	7	0.42
(1,166)	1:12:A:LEU:HD12	1:12:A:LEU:HG	7	0.42
(1,166)	1:12:A:LEU:HD13	1:12:A:LEU:HG	7	0.42
(1,150)	1:15:A:GLY:HA2	1:16:A:GLY:H	5	0.42
(1,69)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.42
(1,50)	1:6:A:ARG:HA	1:6:A:ARG:HB2	7	0.42
(4,30)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	10	0.41
(2,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	10	0.41
(1,430)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	1	0.41
(1,430)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	1	0.41
(1,430)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	1	0.41
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	6	0.41
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	6	0.41
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	6	0.41
(1,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	0.41
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD21	7	0.41
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD22	7	0.41
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD23	7	0.41
(1,388)	1:5:A:VAL:HA	1:8:A:TYR:HB3	1	0.41
(1,381)	1:6:A:ARG:HA	1:9:A:ILE:HB	2	0.41
(1,327)	1:8:A:TYR:HB3	1:9:A:ILE:H	7	0.41
(1,314)	1:8:A:TYR:HD1	1:9:A:ILE:H	4	0.41
(1,314)	1:8:A:TYR:HD2	1:9:A:ILE:H	4	0.41
(1,314)	1:8:A:TYR:HD1	1:9:A:ILE:H	9	0.41
(1,314)	1:8:A:TYR:HD2	1:9:A:ILE:H	9	0.41
(1,298)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	0.41
(1,288)	1:13:A:LYS:H	1:14:A:GLN:H	6	0.41
(1,284)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	4	0.41
(1,278)	1:21:A:ARG:HA	1:21:A:ARG:HB3	1	0.41
(1,254)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:25:A:SER:H	1:25:A:SER:HB2	7	0.41
(1,249)	1:25:A:SER:H	1:25:A:SER:HB3	7	0.41
(1,238)	1:23:A:PRO:HA	1:23:A:PRO:HG2	6	0.41
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD2	9	0.41
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD3	9	0.41
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	2	0.41
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	2	0.41
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	4	0.41
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	4	0.41
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	6	0.41
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	6	0.41
(1,194)	1:18:A:SER:H	1:18:A:SER:HB2	1	0.41
(1,194)	1:18:A:SER:H	1:18:A:SER:HB3	1	0.41
(1,194)	1:18:A:SER:H	1:18:A:SER:HB2	4	0.41
(1,194)	1:18:A:SER:H	1:18:A:SER:HB3	4	0.41
(1,192)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	1	0.41
(1,192)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	4	0.41
(1,192)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	5	0.41
(1,192)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	8	0.41
(1,192)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	9	0.41
(1,192)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.41
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB2	2	0.41
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB3	2	0.41
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB2	6	0.41
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB3	6	0.41
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	1	0.41
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	1	0.41
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	1	0.41
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	5	0.41
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	5	0.41
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	5	0.41
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	5	0.41
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	5	0.41
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	5	0.41
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG2	9	0.41
(1,20)	1:3:A:GLU:HA	1:3:A:GLU:HG3	9	0.41
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	2	0.4
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	2	0.4
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	2	0.4
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	2	0.4
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	2	0.4
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	2	0.4
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	2	0.4
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	2	0.4
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	2	0.4
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	2	0.4
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	2	0.4
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	2	0.4
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	2	0.4
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	2	0.4
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	2	0.4
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	2	0.4
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	2	0.4
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	3	0.4
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	3	0.4
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	3	0.4
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	3	0.4
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	3	0.4
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	3	0.4
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	3	0.4
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	3	0.4
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	3	0.4
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	3	0.4
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	3	0.4
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	3	0.4
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	3	0.4
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	3	0.4
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	3	0.4
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	3	0.4
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	3	0.4
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	3	0.4
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	6	0.4
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	6	0.4
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	6	0.4
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	6	0.4
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	6	0.4
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	6	0.4
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	6	0.4
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	6	0.4
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	6	0.4
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	6	0.4
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	6	0.4
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	6	0.4
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	6	0.4
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	6	0.4
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	6	0.4
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	6	0.4
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	6	0.4
(4,28)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	1	0.4
(4,28)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	1	0.4
(4,28)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	1	0.4
(4,28)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	4	0.4
(4,28)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	4	0.4
(4,28)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	4	0.4
(4,19)	1:11:A:TRP:HA	1:11:A:TRP:HE3	3	0.4
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.4
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.4
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HG3	2	0.4
(3,168)	1:13:A:LYS:H	1:13:A:LYS:HB3	4	0.4
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	2	0.4
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	2	0.4
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	2	0.4
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	2	0.4
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	2	0.4
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	2	0.4
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	2	0.4
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	2	0.4
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	2	0.4
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	2	0.4
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	2	0.4
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	2	0.4
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	2	0.4
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	2	0.4
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	2	0.4
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	2	0.4
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	2	0.4
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	2	0.4
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	3	0.4
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	3	0.4
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	3	0.4
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	3	0.4
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	3	0.4
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	3	0.4
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	3	0.4
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	3	0.4
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	3	0.4
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	3	0.4
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	3	0.4
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	3	0.4
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	3	0.4
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	3	0.4
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	3	0.4
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	3	0.4
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	3	0.4
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	6	0.4
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	6	0.4
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	6	0.4
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	6	0.4
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	6	0.4
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	6	0.4
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	6	0.4
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	6	0.4
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	6	0.4
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	6	0.4
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	6	0.4
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	6	0.4
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	6	0.4
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	6	0.4
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	6	0.4
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	6	0.4
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	6	0.4
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	6	0.4
(2,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	1	0.4
(2,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	1	0.4
(2,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	1	0.4
(2,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	4	0.4
(2,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	4	0.4
(2,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	4	0.4
(2,303)	1:11:A:TRP:HA	1:11:A:TRP:HE3	3	0.4
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.4
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.4
(2,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	4	0.4
(2,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	2	0.4
(1,468)	1:5:A:VAL:HG11	1:6:A:ARG:HA	8	0.4
(1,468)	1:5:A:VAL:HG12	1:6:A:ARG:HA	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:5:A:VAL:HG13	1:6:A:ARG:HA	8	0.4
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:HA	8	0.4
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:HA	8	0.4
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:HA	8	0.4
(1,444)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	10	0.4
(1,444)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	10	0.4
(1,444)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	10	0.4
(1,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	10	0.4
(1,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	10	0.4
(1,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	10	0.4
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	6	0.4
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	6	0.4
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	6	0.4
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	6	0.4
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	6	0.4
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	6	0.4
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	1	0.4
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	1	0.4
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	1	0.4
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	1	0.4
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	1	0.4
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	1	0.4
(1,381)	1:6:A:ARG:HA	1:9:A:ILE:HB	9	0.4
(1,359)	1:8:A:TYR:HD1	1:12:A:LEU:HG	7	0.4
(1,359)	1:8:A:TYR:HD2	1:12:A:LEU:HG	7	0.4
(1,359)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	7	0.4
(1,327)	1:8:A:TYR:HB3	1:9:A:ILE:H	9	0.4
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.4
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	10	0.4
(1,278)	1:21:A:ARG:HA	1:21:A:ARG:HB3	6	0.4
(1,278)	1:21:A:ARG:HA	1:21:A:ARG:HB3	8	0.4
(1,254)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	4	0.4
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD2	10	0.4
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.4
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	4	0.4
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	4	0.4
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	5	0.4
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	5	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	1	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	1	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	3	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	5	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	5	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	7	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	7	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	8	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	8	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	9	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	9	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	10	0.4
(1,207)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	10	0.4
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB2	4	0.4
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB3	4	0.4
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB2	5	0.4
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB3	5	0.4
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB2	10	0.4
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB3	10	0.4
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	2	0.4
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	2	0.4
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	2	0.4
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	4	0.4
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	4	0.4
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	4	0.4
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	7	0.4
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	7	0.4
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	7	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG11	2	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG12	2	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG13	2	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG21	2	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG22	2	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG23	2	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG11	9	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG12	9	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG13	9	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG21	9	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG22	9	0.4
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG23	9	0.4
(1,28)	1:3:A:GLU:HB3	1:4:A:ALA:H	1	0.4
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	5	0.39
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	5	0.39
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	5	0.39
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	5	0.39
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	5	0.39
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	5	0.39
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	5	0.39
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	5	0.39
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	5	0.39
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	5	0.39
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	5	0.39
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	5	0.39
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	5	0.39
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	5	0.39
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	5	0.39
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	5	0.39
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	5	0.39
(4,33)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	8	0.39
(4,33)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	8	0.39
(4,28)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	5	0.39
(4,28)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	5	0.39
(4,28)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	5	0.39
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.39
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.39
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.39
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.39
(4,18)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.39
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG2	5	0.39
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG3	5	0.39
(3,400)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	4	0.39
(3,400)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	4	0.39
(3,400)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	4	0.39
(3,360)	1:15:A:GLY:HA3	1:18:A:SER:HB3	2	0.39
(3,318)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.39
(3,247)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	8	0.39
(3,247)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	10	0.39
(3,168)	1:13:A:LYS:H	1:13:A:LYS:HB3	2	0.39
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	5	0.39
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	5	0.39
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	5	0.39
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	5	0.39
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	5	0.39
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	5	0.39
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	5	0.39
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	5	0.39
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	5	0.39
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	5	0.39
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	5	0.39
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	5	0.39
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	5	0.39
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	5	0.39
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	5	0.39
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	5	0.39
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	5	0.39
(2,434)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	4	0.39
(2,434)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	4	0.39
(2,434)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	4	0.39
(2,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	8	0.39
(2,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	8	0.39
(2,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	5	0.39
(2,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	5	0.39
(2,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	5	0.39
(2,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	2	0.39
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.39
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.39
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.39
(2,340)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.39
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.39
(2,294)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.39
(2,264)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	8	0.39
(2,264)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	10	0.39
(2,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	2	0.39
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG2	5	0.39
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG3	5	0.39
(1,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	0.39
(1,338)	1:21:A:ARG:H	1:21:A:ARG:HB2	2	0.39
(1,284)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	1	0.39
(1,261)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	6	0.39
(1,256)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	8	0.39
(1,254)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	1	0.39
(1,254)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	5	0.39
(1,254)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	9	0.39
(1,249)	1:25:A:SER:H	1:25:A:SER:HB2	2	0.39
(1,249)	1:25:A:SER:H	1:25:A:SER:HB3	2	0.39
(1,238)	1:23:A:PRO:HA	1:23:A:PRO:HG2	3	0.39
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	1	0.39
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	8	0.39
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	8	0.39
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.39
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	10	0.39
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	5	0.39
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	5	0.39
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	8	0.39
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	8	0.39
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB2	9	0.39
(1,191)	1:14:A:GLN:HA	1:14:A:GLN:HB3	9	0.39
(1,153)	1:16:A:GLY:H	1:16:A:GLY:HA3	7	0.39
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	1	0.39
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	1	0.39
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	1	0.39
(4,40)	1:3:A:GLU:HG2	1:6:A:ARG:H	3	0.38
(4,40)	1:3:A:GLU:HG3	1:6:A:ARG:H	3	0.38
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	4	0.38
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	4	0.38
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	4	0.38
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	4	0.38
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	4	0.38
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	4	0.38
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	4	0.38
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	4	0.38
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	4	0.38
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	4	0.38
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	4	0.38
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	4	0.38
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	4	0.38
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	4	0.38
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	4	0.38
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	4	0.38
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	4	0.38
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	4	0.38
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	10	0.38
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	10	0.38
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	10	0.38
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	10	0.38
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	10	0.38
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	10	0.38
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	10	0.38
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	10	0.38
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	10	0.38
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	10	0.38
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	10	0.38
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	10	0.38
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	10	0.38
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	10	0.38
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	10	0.38
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	10	0.38
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	10	0.38
(4,33)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	7	0.38
(4,33)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	7	0.38
(4,13)	1:11:A:TRP:H	1:11:A:TRP:HD1	8	0.38
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG2	6	0.38
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG3	6	0.38
(3,394)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	8	0.38
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	6	0.38
(3,247)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	1	0.38
(3,247)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	3	0.38
(3,247)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	4	0.38
(3,247)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	5	0.38
(3,247)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	7	0.38
(3,247)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	9	0.38
(3,168)	1:13:A:LYS:H	1:13:A:LYS:HB3	3	0.38
(3,168)	1:13:A:LYS:H	1:13:A:LYS:HB3	5	0.38
(2,461)	1:3:A:GLU:HG2	1:6:A:ARG:H	3	0.38
(2,461)	1:3:A:GLU:HG3	1:6:A:ARG:H	3	0.38
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	4	0.38
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	4	0.38
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	4	0.38
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	4	0.38
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	4	0.38
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	4	0.38
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	4	0.38
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	4	0.38
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	4	0.38
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	4	0.38
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	4	0.38
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	4	0.38
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	4	0.38
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	4	0.38
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	4	0.38
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	4	0.38
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	4	0.38
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	10	0.38
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	10	0.38
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	10	0.38
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	10	0.38
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	10	0.38
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	10	0.38
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	10	0.38
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	10	0.38
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	10	0.38
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	10	0.38
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	10	0.38
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	10	0.38
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	10	0.38
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	10	0.38
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	10	0.38
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	10	0.38
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	10	0.38
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	10	0.38
(2,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	8	0.38
(2,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	7	0.38
(2,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	7	0.38
(2,333)	1:12:A:LEU:HB3	1:13:A:LYS:H	6	0.38
(2,264)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	1	0.38
(2,264)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	3	0.38
(2,264)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	4	0.38
(2,264)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	5	0.38
(2,264)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	7	0.38
(2,264)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	9	0.38
(2,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	3	0.38
(2,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	5	0.38
(2,139)	1:11:A:TRP:H	1:11:A:TRP:HD1	8	0.38
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG2	6	0.38
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG3	6	0.38
(1,468)	1:5:A:VAL:HG11	1:6:A:ARG:HA	4	0.38
(1,468)	1:5:A:VAL:HG12	1:6:A:ARG:HA	4	0.38
(1,468)	1:5:A:VAL:HG13	1:6:A:ARG:HA	4	0.38
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:HA	4	0.38
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:HA	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:HA	4	0.38
(1,468)	1:5:A:VAL:HG11	1:6:A:ARG:HA	5	0.38
(1,468)	1:5:A:VAL:HG12	1:6:A:ARG:HA	5	0.38
(1,468)	1:5:A:VAL:HG13	1:6:A:ARG:HA	5	0.38
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:HA	5	0.38
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:HA	5	0.38
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:HA	5	0.38
(1,385)	1:7:A:LEU:HD11	1:8:A:TYR:HA	5	0.38
(1,385)	1:7:A:LEU:HD12	1:8:A:TYR:HA	5	0.38
(1,385)	1:7:A:LEU:HD13	1:8:A:TYR:HA	5	0.38
(1,376)	1:8:A:TYR:HA	1:24:A:PRO:HD3	7	0.38
(1,376)	1:8:A:TYR:HA	1:24:A:PRO:HD3	8	0.38
(1,338)	1:21:A:ARG:H	1:21:A:ARG:HB2	1	0.38
(1,338)	1:21:A:ARG:H	1:21:A:ARG:HB2	3	0.38
(1,313)	1:11:A:TRP:HE3	1:12:A:LEU:H	3	0.38
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	2	0.38
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	2	0.38
(1,278)	1:21:A:ARG:HA	1:21:A:ARG:HB3	4	0.38
(1,254)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	2	0.38
(1,238)	1:23:A:PRO:HA	1:23:A:PRO:HG2	1	0.38
(1,238)	1:23:A:PRO:HA	1:23:A:PRO:HG2	2	0.38
(1,238)	1:23:A:PRO:HA	1:23:A:PRO:HG2	5	0.38
(1,238)	1:23:A:PRO:HA	1:23:A:PRO:HG2	10	0.38
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	2	0.38
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	2	0.38
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	3	0.38
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	3	0.38
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	6	0.38
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	6	0.38
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	7	0.38
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	7	0.38
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	9	0.38
(1,223)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	9	0.38
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	4	0.38
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	4	0.38
(1,198)	1:19:A:SER:H	1:19:A:SER:HB3	9	0.38
(1,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	1	0.38
(1,167)	1:12:A:LEU:HD21	1:12:A:LEU:HG	1	0.38
(1,167)	1:12:A:LEU:HD22	1:12:A:LEU:HG	1	0.38
(1,167)	1:12:A:LEU:HD23	1:12:A:LEU:HG	1	0.38
(1,167)	1:12:A:LEU:HD21	1:12:A:LEU:HG	2	0.38
(1,167)	1:12:A:LEU:HD22	1:12:A:LEU:HG	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	1:12:A:LEU:HD23	1:12:A:LEU:HG	2	0.38
(1,167)	1:12:A:LEU:HD21	1:12:A:LEU:HG	4	0.38
(1,167)	1:12:A:LEU:HD22	1:12:A:LEU:HG	4	0.38
(1,167)	1:12:A:LEU:HD23	1:12:A:LEU:HG	4	0.38
(1,153)	1:16:A:GLY:H	1:16:A:GLY:HA3	1	0.38
(1,153)	1:16:A:GLY:H	1:16:A:GLY:HA3	2	0.38
(1,153)	1:16:A:GLY:H	1:16:A:GLY:HA3	3	0.38
(1,153)	1:16:A:GLY:H	1:16:A:GLY:HA3	4	0.38
(1,153)	1:16:A:GLY:H	1:16:A:GLY:HA3	6	0.38
(1,153)	1:16:A:GLY:H	1:16:A:GLY:HA3	8	0.38
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	4	0.38
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	4	0.38
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	4	0.38
(1,18)	1:3:A:GLU:HA	1:3:A:GLU:HB2	1	0.38
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	8	0.37
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	8	0.37
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	8	0.37
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	8	0.37
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	8	0.37
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	8	0.37
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	8	0.37
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	8	0.37
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	8	0.37
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	8	0.37
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	8	0.37
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	8	0.37
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	8	0.37
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	8	0.37
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	8	0.37
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	8	0.37
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	8	0.37
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	8	0.37
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	1	0.37
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	1	0.37
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	1	0.37
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HG3	8	0.37
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.37
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.37
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.37
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.37
(3,400)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	1	0.37
(3,400)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,400)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	1	0.37
(3,247)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	2	0.37
(3,114)	1:10:A:GLN:H	1:10:A:GLN:HB2	6	0.37
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	8	0.37
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	8	0.37
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	8	0.37
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	8	0.37
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	8	0.37
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	8	0.37
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	8	0.37
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	8	0.37
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	8	0.37
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	8	0.37
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	8	0.37
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	8	0.37
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	8	0.37
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	8	0.37
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	8	0.37
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	8	0.37
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	8	0.37
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	8	0.37
(2,434)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	1	0.37
(2,434)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	1	0.37
(2,434)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	1	0.37
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	1	0.37
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	1	0.37
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	1	0.37
(2,264)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	2	0.37
(2,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	6	0.37
(2,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	8	0.37
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.37
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.37
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.37
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.37
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	6	0.37
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB3	6	0.37
(1,338)	1:21:A:ARG:H	1:21:A:ARG:HB2	8	0.37
(1,327)	1:8:A:TYR:HB3	1:9:A:ILE:H	1	0.37
(1,327)	1:8:A:TYR:HB3	1:9:A:ILE:H	4	0.37
(1,278)	1:21:A:ARG:HA	1:21:A:ARG:HB3	2	0.37
(1,238)	1:23:A:PRO:HA	1:23:A:PRO:HG2	4	0.37
(1,238)	1:23:A:PRO:HA	1:23:A:PRO:HG2	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,238)	1:23:A:PRO:HA	1:23:A:PRO:HG2	9	0.37
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD2	2	0.37
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD3	2	0.37
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD2	7	0.37
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD3	7	0.37
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	1	0.37
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	1	0.37
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	9	0.37
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	9	0.37
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	10	0.37
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.37
(1,167)	1:12:A:LEU:HD21	1:12:A:LEU:HG	5	0.37
(1,167)	1:12:A:LEU:HD22	1:12:A:LEU:HG	5	0.37
(1,167)	1:12:A:LEU:HD23	1:12:A:LEU:HG	5	0.37
(1,167)	1:12:A:LEU:HD21	1:12:A:LEU:HG	6	0.37
(1,167)	1:12:A:LEU:HD22	1:12:A:LEU:HG	6	0.37
(1,167)	1:12:A:LEU:HD23	1:12:A:LEU:HG	6	0.37
(1,167)	1:12:A:LEU:HD21	1:12:A:LEU:HG	7	0.37
(1,167)	1:12:A:LEU:HD22	1:12:A:LEU:HG	7	0.37
(1,167)	1:12:A:LEU:HD23	1:12:A:LEU:HG	7	0.37
(1,167)	1:12:A:LEU:HD21	1:12:A:LEU:HG	9	0.37
(1,167)	1:12:A:LEU:HD22	1:12:A:LEU:HG	9	0.37
(1,167)	1:12:A:LEU:HD23	1:12:A:LEU:HG	9	0.37
(1,167)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.37
(1,167)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.37
(1,167)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.37
(1,96)	1:8:A:TYR:HA	1:8:A:TYR:HB2	10	0.37
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	9	0.37
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	9	0.37
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	9	0.37
(1,79)	1:7:A:LEU:HA	1:7:A:LEU:HB3	3	0.37
(1,79)	1:7:A:LEU:HA	1:7:A:LEU:HB3	5	0.37
(1,79)	1:7:A:LEU:HA	1:7:A:LEU:HB3	6	0.37
(1,79)	1:7:A:LEU:HA	1:7:A:LEU:HB3	7	0.37
(1,79)	1:7:A:LEU:HA	1:7:A:LEU:HB3	9	0.37
(1,79)	1:7:A:LEU:HA	1:7:A:LEU:HB3	10	0.37
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.36
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.36
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.36
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	4	0.36
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	4	0.36
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	5	0.36
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	5	0.36
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	5	0.36
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG2	8	0.36
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG3	8	0.36
(3,114)	1:10:A:GLN:H	1:10:A:GLN:HB2	1	0.36
(3,114)	1:10:A:GLN:H	1:10:A:GLN:HB2	5	0.36
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.36
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.36
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.36
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	4	0.36
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	4	0.36
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	4	0.36
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	5	0.36
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	5	0.36
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	5	0.36
(2,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	1	0.36
(2,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	5	0.36
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG2	8	0.36
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG3	8	0.36
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	10	0.36
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	10	0.36
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	10	0.36
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	10	0.36
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	10	0.36
(1,483)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	10	0.36
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	10	0.36
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	10	0.36
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	10	0.36
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	10	0.36
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	10	0.36
(1,483)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	10	0.36
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB2	10	0.36
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB3	10	0.36
(1,468)	1:5:A:VAL:HG11	1:6:A:ARG:HA	6	0.36
(1,468)	1:5:A:VAL:HG12	1:6:A:ARG:HA	6	0.36
(1,468)	1:5:A:VAL:HG13	1:6:A:ARG:HA	6	0.36
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:HA	6	0.36
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:HA	6	0.36
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:HA	6	0.36
(1,468)	1:5:A:VAL:HG11	1:6:A:ARG:HA	9	0.36
(1,468)	1:5:A:VAL:HG12	1:6:A:ARG:HA	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:5:A:VAL:HG13	1:6:A:ARG:HA	9	0.36
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:HA	9	0.36
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:HA	9	0.36
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:HA	9	0.36
(1,444)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	8	0.36
(1,444)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	8	0.36
(1,444)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	8	0.36
(1,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	8	0.36
(1,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	8	0.36
(1,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	8	0.36
(1,430)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	4	0.36
(1,430)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	4	0.36
(1,430)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	4	0.36
(1,430)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	7	0.36
(1,430)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	7	0.36
(1,430)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	7	0.36
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	1	0.36
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	1	0.36
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	1	0.36
(1,338)	1:21:A:ARG:H	1:21:A:ARG:HB2	6	0.36
(1,313)	1:11:A:TRP:HE3	1:12:A:LEU:H	8	0.36
(1,284)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	3	0.36
(1,284)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	7	0.36
(1,279)	1:21:A:ARG:HA	1:21:A:ARG:HG2	5	0.36
(1,278)	1:21:A:ARG:HA	1:21:A:ARG:HB3	3	0.36
(1,259)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	6	0.36
(1,254)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	7	0.36
(1,249)	1:25:A:SER:H	1:25:A:SER:HB2	3	0.36
(1,249)	1:25:A:SER:H	1:25:A:SER:HB3	3	0.36
(1,238)	1:23:A:PRO:HA	1:23:A:PRO:HG2	8	0.36
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD2	3	0.36
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD3	3	0.36
(1,217)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	1	0.36
(1,217)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	2	0.36
(1,217)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	3	0.36
(1,217)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	4	0.36
(1,217)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	5	0.36
(1,217)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	6	0.36
(1,217)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	7	0.36
(1,217)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	8	0.36
(1,217)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	9	0.36
(1,217)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	7	0.36
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	7	0.36
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	7	0.36
(1,167)	1:12:A:LEU:HD21	1:12:A:LEU:HG	3	0.36
(1,167)	1:12:A:LEU:HD22	1:12:A:LEU:HG	3	0.36
(1,167)	1:12:A:LEU:HD23	1:12:A:LEU:HG	3	0.36
(1,167)	1:12:A:LEU:HD21	1:12:A:LEU:HG	8	0.36
(1,167)	1:12:A:LEU:HD22	1:12:A:LEU:HG	8	0.36
(1,167)	1:12:A:LEU:HD23	1:12:A:LEU:HG	8	0.36
(1,153)	1:16:A:GLY:H	1:16:A:GLY:HA3	5	0.36
(1,79)	1:7:A:LEU:HA	1:7:A:LEU:HB3	1	0.36
(1,79)	1:7:A:LEU:HA	1:7:A:LEU:HB3	2	0.36
(1,79)	1:7:A:LEU:HA	1:7:A:LEU:HB3	4	0.36
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG11	5	0.36
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG12	5	0.36
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG13	5	0.36
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG21	5	0.36
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG22	5	0.36
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG23	5	0.36
(1,18)	1:3:A:GLU:HA	1:3:A:GLU:HB2	2	0.36
(1,18)	1:3:A:GLU:HA	1:3:A:GLU:HB2	9	0.36
(1,10)	1:15:A:GLY:H	1:15:A:GLY:HA2	3	0.36
(4,28)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	10	0.35
(4,28)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	10	0.35
(4,28)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	10	0.35
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	9	0.35
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	9	0.35
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	9	0.35
(4,21)	1:8:A:TYR:HB2	1:9:A:ILE:H	6	0.35
(4,21)	1:8:A:TYR:HB2	1:9:A:ILE:H	7	0.35
(4,13)	1:11:A:TRP:H	1:11:A:TRP:HD1	1	0.35
(4,13)	1:11:A:TRP:H	1:11:A:TRP:HD1	3	0.35
(4,13)	1:11:A:TRP:H	1:11:A:TRP:HD1	10	0.35
(3,393)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	4	0.35
(3,318)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.35
(3,295)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.35
(2,427)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	4	0.35
(2,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	10	0.35
(2,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	10	0.35
(2,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	10	0.35
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	9	0.35
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	9	0.35
(2,340)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.35
(2,325)	1:8:A:TYR:HB2	1:9:A:ILE:H	6	0.35
(2,325)	1:8:A:TYR:HB2	1:9:A:ILE:H	7	0.35
(2,315)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.35
(2,139)	1:11:A:TRP:H	1:11:A:TRP:HD1	1	0.35
(2,139)	1:11:A:TRP:H	1:11:A:TRP:HD1	3	0.35
(2,139)	1:11:A:TRP:H	1:11:A:TRP:HD1	10	0.35
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB2	5	0.35
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB3	5	0.35
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB2	9	0.35
(1,479)	1:1:A:GLU:HA	1:1:A:GLU:HB3	9	0.35
(1,468)	1:5:A:VAL:HG11	1:6:A:ARG:HA	2	0.35
(1,468)	1:5:A:VAL:HG12	1:6:A:ARG:HA	2	0.35
(1,468)	1:5:A:VAL:HG13	1:6:A:ARG:HA	2	0.35
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:HA	2	0.35
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:HA	2	0.35
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:HA	2	0.35
(1,435)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	6	0.35
(1,435)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	6	0.35
(1,435)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	6	0.35
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	0.35
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	0.35
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	0.35
(1,416)	1:8:A:TYR:HB2	1:24:A:PRO:HD2	5	0.35
(1,388)	1:5:A:VAL:HA	1:8:A:TYR:HB3	8	0.35
(1,327)	1:8:A:TYR:HB3	1:9:A:ILE:H	2	0.35
(1,322)	1:18:A:SER:H	1:20:A:GLY:H	1	0.35
(1,288)	1:13:A:LYS:H	1:14:A:GLN:H	3	0.35
(1,232)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	6	0.35
(1,232)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	6	0.35
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	2	0.35
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	2	0.35
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	7	0.35
(1,177)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	7	0.35
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	7	0.35
(1,177)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	7	0.35
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	9	0.35
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	9	0.35
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	9	0.35
(1,155)	1:12:A:LEU:HA	1:16:A:GLY:H	2	0.35
(1,143)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	2	0.35
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	2	0.35
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	2	0.35
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	3	0.35
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	3	0.35
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	3	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG11	4	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG12	4	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG13	4	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG21	4	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG22	4	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG23	4	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG11	6	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG12	6	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG13	6	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG21	6	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG22	6	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG23	6	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG11	8	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG12	8	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG13	8	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG21	8	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG22	8	0.35
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG23	8	0.35
(1,18)	1:3:A:GLU:HA	1:3:A:GLU:HB2	3	0.35
(1,18)	1:3:A:GLU:HA	1:3:A:GLU:HB2	7	0.35
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	7	0.34
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	7	0.34
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	7	0.34
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	7	0.34
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	7	0.34
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	7	0.34
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	7	0.34
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	7	0.34
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	7	0.34
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	7	0.34
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	7	0.34
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	7	0.34
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	7	0.34
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	7	0.34
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	7	0.34
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	7	0.34
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	7	0.34
(4,31)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	1	0.34
(4,31)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	9	0.34
(4,13)	1:11:A:TRP:H	1:11:A:TRP:HD1	2	0.34
(4,13)	1:11:A:TRP:H	1:11:A:TRP:HD1	4	0.34
(4,13)	1:11:A:TRP:H	1:11:A:TRP:HD1	7	0.34
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG2	7	0.34
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG3	7	0.34
(3,318)	1:21:A:ARG:H	1:21:A:ARG:HB3	1	0.34
(3,318)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.34
(3,176)	1:14:A:GLN:HA	1:14:A:GLN:HG2	2	0.34
(3,176)	1:14:A:GLN:HA	1:14:A:GLN:HG2	6	0.34
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	7	0.34
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	7	0.34
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	7	0.34
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	7	0.34
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	7	0.34
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	7	0.34
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	7	0.34
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	7	0.34
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	7	0.34
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	7	0.34
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	7	0.34
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	7	0.34
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	7	0.34
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	7	0.34
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	7	0.34
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	7	0.34
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	7	0.34
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	7	0.34
(2,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	1	0.34
(2,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	9	0.34
(2,340)	1:21:A:ARG:H	1:21:A:ARG:HB3	1	0.34
(2,340)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.34
(2,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	2	0.34
(2,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	6	0.34
(2,139)	1:11:A:TRP:H	1:11:A:TRP:HD1	2	0.34
(2,139)	1:11:A:TRP:H	1:11:A:TRP:HD1	4	0.34
(2,139)	1:11:A:TRP:H	1:11:A:TRP:HD1	7	0.34
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG2	7	0.34
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG3	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:5:A:VAL:HA	1:8:A:TYR:HD1	3	0.34
(1,473)	1:5:A:VAL:HA	1:8:A:TYR:HD2	3	0.34
(1,468)	1:5:A:VAL:HG11	1:6:A:ARG:HA	3	0.34
(1,468)	1:5:A:VAL:HG12	1:6:A:ARG:HA	3	0.34
(1,468)	1:5:A:VAL:HG13	1:6:A:ARG:HA	3	0.34
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:HA	3	0.34
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:HA	3	0.34
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:HA	3	0.34
(1,468)	1:5:A:VAL:HG11	1:6:A:ARG:HA	10	0.34
(1,468)	1:5:A:VAL:HG12	1:6:A:ARG:HA	10	0.34
(1,468)	1:5:A:VAL:HG13	1:6:A:ARG:HA	10	0.34
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:HA	10	0.34
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:HA	10	0.34
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:HA	10	0.34
(1,465)	1:3:A:GLU:HA	1:6:A:ARG:HB3	6	0.34
(1,412)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	3	0.34
(1,329)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	9	0.34
(1,329)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	9	0.34
(1,314)	1:8:A:TYR:HD1	1:9:A:ILE:H	6	0.34
(1,314)	1:8:A:TYR:HD2	1:9:A:ILE:H	6	0.34
(1,284)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	10	0.34
(1,283)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	7	0.34
(1,283)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	10	0.34
(1,232)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	2	0.34
(1,232)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	2	0.34
(1,232)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	4	0.34
(1,232)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	4	0.34
(1,232)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	5	0.34
(1,232)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	5	0.34
(1,232)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	7	0.34
(1,232)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	7	0.34
(1,232)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	8	0.34
(1,232)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	8	0.34
(1,232)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	10	0.34
(1,232)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.34
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	3	0.34
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	3	0.34
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	6	0.34
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	6	0.34
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	7	0.34
(1,222)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	7	0.34
(1,209)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:16:A:GLY:H	1:16:A:GLY:HA3	10	0.34
(1,143)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	1	0.34
(1,143)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	2	0.34
(1,143)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	3	0.34
(1,143)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	4	0.34
(1,143)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	5	0.34
(1,143)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	6	0.34
(1,143)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	8	0.34
(1,143)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	9	0.34
(1,143)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.34
(1,96)	1:8:A:TYR:HA	1:8:A:TYR:HB2	3	0.34
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	6	0.34
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	6	0.34
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	6	0.34
(1,79)	1:7:A:LEU:HA	1:7:A:LEU:HB3	8	0.34
(1,18)	1:3:A:GLU:HA	1:3:A:GLU:HB2	8	0.34
(4,40)	1:3:A:GLU:HG2	1:6:A:ARG:H	1	0.33
(4,40)	1:3:A:GLU:HG3	1:6:A:ARG:H	1	0.33
(4,40)	1:3:A:GLU:HG2	1:6:A:ARG:H	8	0.33
(4,40)	1:3:A:GLU:HG3	1:6:A:ARG:H	8	0.33
(4,31)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	5	0.33
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	6	0.33
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	6	0.33
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	6	0.33
(4,13)	1:11:A:TRP:H	1:11:A:TRP:HD1	9	0.33
(3,382)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	1	0.33
(3,331)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	3	0.33
(3,318)	1:21:A:ARG:H	1:21:A:ARG:HB3	9	0.33
(2,461)	1:3:A:GLU:HG2	1:6:A:ARG:H	1	0.33
(2,461)	1:3:A:GLU:HG3	1:6:A:ARG:H	1	0.33
(2,461)	1:3:A:GLU:HG2	1:6:A:ARG:H	8	0.33
(2,461)	1:3:A:GLU:HG3	1:6:A:ARG:H	8	0.33
(2,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	5	0.33
(2,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	1	0.33
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	6	0.33
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	6	0.33
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	6	0.33
(2,353)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	3	0.33
(2,340)	1:21:A:ARG:H	1:21:A:ARG:HB3	9	0.33
(2,139)	1:11:A:TRP:H	1:11:A:TRP:HD1	9	0.33
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	2	0.33
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	2	0.33
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	2	0.33
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	2	0.33
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	2	0.33
(1,430)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	8	0.33
(1,430)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	8	0.33
(1,430)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	8	0.33
(1,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	8	0.33
(1,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	0.33
(1,338)	1:21:A:ARG:H	1:21:A:ARG:HB2	4	0.33
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	1	0.33
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	1	0.33
(1,283)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	3	0.33
(1,283)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	5	0.33
(1,283)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	8	0.33
(1,232)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	1	0.33
(1,232)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	1	0.33
(1,232)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	3	0.33
(1,232)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	3	0.33
(1,232)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	9	0.33
(1,232)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	9	0.33
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD2	6	0.33
(1,229)	1:22:A:PRO:HA	1:23:A:PRO:HD3	6	0.33
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	6	0.33
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	6	0.33
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	6	0.33
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	10	0.33
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	10	0.33
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	10	0.33
(1,69)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.33
(1,18)	1:3:A:GLU:HA	1:3:A:GLU:HB2	6	0.33
(1,18)	1:3:A:GLU:HA	1:3:A:GLU:HB2	10	0.33
(4,31)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	10	0.32
(4,21)	1:8:A:TYR:HB2	1:9:A:ILE:H	8	0.32
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HG3	1	0.32
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG2	2	0.32
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG3	2	0.32
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG2	3	0.32
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG3	3	0.32
(3,400)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	2	0.32
(3,400)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	2	0.32
(3,400)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,318)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.32
(3,318)	1:21:A:ARG:H	1:21:A:ARG:HB3	4	0.32
(3,318)	1:21:A:ARG:H	1:21:A:ARG:HB3	8	0.32
(3,295)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.32
(2,434)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	2	0.32
(2,434)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	2	0.32
(2,434)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	2	0.32
(2,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	10	0.32
(2,340)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.32
(2,340)	1:21:A:ARG:H	1:21:A:ARG:HB3	4	0.32
(2,340)	1:21:A:ARG:H	1:21:A:ARG:HB3	8	0.32
(2,325)	1:8:A:TYR:HB2	1:9:A:ILE:H	8	0.32
(2,315)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.32
(2,70)	1:6:A:ARG:H	1:6:A:ARG:HG3	1	0.32
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG2	2	0.32
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG3	2	0.32
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG2	3	0.32
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG3	3	0.32
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB1	4	0.32
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB2	4	0.32
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB3	4	0.32
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB1	4	0.32
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB2	4	0.32
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB3	4	0.32
(1,444)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	9	0.32
(1,444)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	9	0.32
(1,444)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	9	0.32
(1,444)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	9	0.32
(1,444)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	9	0.32
(1,444)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	9	0.32
(1,441)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	5	0.32
(1,441)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	5	0.32
(1,441)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	5	0.32
(1,378)	1:8:A:TYR:HA	1:24:A:PRO:HD2	8	0.32
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	4	0.32
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	4	0.32
(1,263)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	1	0.32
(1,263)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	2	0.32
(1,263)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	4	0.32
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG2	5	0.32
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG3	5	0.32
(1,63)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	2	0.32
(1,63)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	3	0.32
(1,63)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	4	0.32
(1,63)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	8	0.32
(1,63)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	9	0.32
(1,63)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.32
(1,18)	1:3:A:GLU:HA	1:3:A:GLU:HB2	4	0.32
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	1	0.31
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	1	0.31
(4,35)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	1	0.31
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	1	0.31
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	1	0.31
(4,35)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	1	0.31
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	1	0.31
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	1	0.31
(4,35)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	1	0.31
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	1	0.31
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	1	0.31
(4,35)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	1	0.31
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	1	0.31
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	1	0.31
(4,35)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	1	0.31
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	1	0.31
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	1	0.31
(4,35)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	1	0.31
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	3	0.31
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	3	0.31
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	3	0.31
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	7	0.31
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	7	0.31
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	7	0.31
(4,13)	1:11:A:TRP:H	1:11:A:TRP:HD1	5	0.31
(3,393)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	5	0.31
(3,318)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.31
(3,295)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.31
(3,295)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.31
(3,295)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.31
(3,295)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.31
(3,295)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.31
(3,176)	1:14:A:GLN:HA	1:14:A:GLN:HG2	10	0.31
(3,114)	1:10:A:GLN:H	1:10:A:GLN:HB2	9	0.31
(3,46)	1:6:A:ARG:HA	1:6:A:ARG:HD3	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	1	0.31
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	1	0.31
(2,446)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	1	0.31
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	1	0.31
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	1	0.31
(2,446)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	1	0.31
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	1	0.31
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	1	0.31
(2,446)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	1	0.31
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	1	0.31
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	1	0.31
(2,446)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	1	0.31
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	1	0.31
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	1	0.31
(2,446)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	1	0.31
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	1	0.31
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	1	0.31
(2,446)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	1	0.31
(2,427)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	5	0.31
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	3	0.31
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	3	0.31
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	3	0.31
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	7	0.31
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	7	0.31
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	7	0.31
(2,340)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.31
(2,315)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.31
(2,315)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.31
(2,315)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.31
(2,315)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.31
(2,315)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.31
(2,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	10	0.31
(2,139)	1:11:A:TRP:H	1:11:A:TRP:HD1	5	0.31
(2,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	9	0.31
(2,49)	1:6:A:ARG:HA	1:6:A:ARG:HD3	5	0.31
(1,465)	1:3:A:GLU:HA	1:6:A:ARG:HB3	7	0.31
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	4	0.31
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB3	4	0.31
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	9	0.31
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	9	0.31
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	9	0.31
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	9	0.31
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	9	0.31
(1,413)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	0.31
(1,384)	1:7:A:LEU:HD11	1:8:A:TYR:HA	8	0.31
(1,384)	1:7:A:LEU:HD12	1:8:A:TYR:HA	8	0.31
(1,384)	1:7:A:LEU:HD13	1:8:A:TYR:HA	8	0.31
(1,381)	1:6:A:ARG:HA	1:9:A:ILE:HB	7	0.31
(1,376)	1:8:A:TYR:HA	1:24:A:PRO:HD3	1	0.31
(1,359)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	0.31
(1,359)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	0.31
(1,359)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	5	0.31
(1,356)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	1	0.31
(1,327)	1:8:A:TYR:HB3	1:9:A:ILE:H	5	0.31
(1,278)	1:21:A:ARG:HA	1:21:A:ARG:HB3	5	0.31
(1,278)	1:21:A:ARG:HA	1:21:A:ARG:HB3	9	0.31
(1,254)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	8	0.31
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	2	0.31
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	2	0.31
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG2	6	0.31
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG3	6	0.31
(1,194)	1:18:A:SER:H	1:18:A:SER:HB2	9	0.31
(1,194)	1:18:A:SER:H	1:18:A:SER:HB3	9	0.31
(1,85)	1:7:A:LEU:HD11	1:7:A:LEU:HG	8	0.31
(1,85)	1:7:A:LEU:HD12	1:7:A:LEU:HG	8	0.31
(1,85)	1:7:A:LEU:HD13	1:7:A:LEU:HG	8	0.31
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	8	0.31
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	8	0.31
(1,83)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	8	0.31
(1,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	2	0.31
(1,63)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	5	0.31
(1,63)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	6	0.31
(1,63)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	7	0.31
(1,56)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	9	0.31
(1,18)	1:3:A:GLU:HA	1:3:A:GLU:HB2	5	0.31
(4,31)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	3	0.3
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG2	9	0.3
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG3	9	0.3
(3,295)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.3
(3,295)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.3
(2,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	3	0.3
(2,315)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.3
(2,315)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG2	9	0.3
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG3	9	0.3
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.3
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB3	2	0.3
(1,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	2	0.3
(1,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	5	0.3
(1,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	1	0.3
(1,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	1	0.3
(1,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	1	0.3
(1,288)	1:13:A:LYS:H	1:14:A:GLN:H	4	0.3
(1,278)	1:21:A:ARG:HA	1:21:A:ARG:HB3	10	0.3
(1,267)	1:24:A:PRO:HA	1:24:A:PRO:HB3	5	0.3
(1,267)	1:24:A:PRO:HA	1:24:A:PRO:HB3	7	0.3
(1,267)	1:24:A:PRO:HA	1:24:A:PRO:HB3	9	0.3
(1,263)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	5	0.3
(1,263)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	6	0.3
(1,263)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	7	0.3
(1,263)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	8	0.3
(1,225)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	6	0.3
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	1	0.3
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	1	0.3
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	4	0.3
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	4	0.3
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	6	0.3
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	6	0.3
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	7	0.3
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	7	0.3
(1,85)	1:7:A:LEU:HD11	1:7:A:LEU:HG	2	0.3
(1,85)	1:7:A:LEU:HD12	1:7:A:LEU:HG	2	0.3
(1,85)	1:7:A:LEU:HD13	1:7:A:LEU:HG	2	0.3
(1,85)	1:7:A:LEU:HD11	1:7:A:LEU:HG	3	0.3
(1,85)	1:7:A:LEU:HD12	1:7:A:LEU:HG	3	0.3
(1,85)	1:7:A:LEU:HD13	1:7:A:LEU:HG	3	0.3
(1,85)	1:7:A:LEU:HD11	1:7:A:LEU:HG	4	0.3
(1,85)	1:7:A:LEU:HD12	1:7:A:LEU:HG	4	0.3
(1,85)	1:7:A:LEU:HD13	1:7:A:LEU:HG	4	0.3
(1,85)	1:7:A:LEU:HD11	1:7:A:LEU:HG	7	0.3
(1,85)	1:7:A:LEU:HD12	1:7:A:LEU:HG	7	0.3
(1,85)	1:7:A:LEU:HD13	1:7:A:LEU:HG	7	0.3
(1,85)	1:7:A:LEU:HD11	1:7:A:LEU:HG	10	0.3
(1,85)	1:7:A:LEU:HD12	1:7:A:LEU:HG	10	0.3
(1,85)	1:7:A:LEU:HD13	1:7:A:LEU:HG	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	4	0.3
(1,56)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	1	0.3
(4,40)	1:3:A:GLU:HG2	1:6:A:ARG:H	4	0.29
(4,40)	1:3:A:GLU:HG3	1:6:A:ARG:H	4	0.29
(3,295)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.29
(3,114)	1:10:A:GLN:H	1:10:A:GLN:HB2	2	0.29
(2,461)	1:3:A:GLU:HG2	1:6:A:ARG:H	4	0.29
(2,461)	1:3:A:GLU:HG3	1:6:A:ARG:H	4	0.29
(2,315)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.29
(2,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	2	0.29
(1,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	9	0.29
(1,431)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	3	0.29
(1,431)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	3	0.29
(1,431)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	3	0.29
(1,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	5	0.29
(1,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	5	0.29
(1,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	5	0.29
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	7	0.29
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	7	0.29
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	7	0.29
(1,399)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	4	0.29
(1,399)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	4	0.29
(1,399)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	4	0.29
(1,399)	1:5:A:VAL:HG21	1:8:A:TYR:HB3	4	0.29
(1,399)	1:5:A:VAL:HG22	1:8:A:TYR:HB3	4	0.29
(1,399)	1:5:A:VAL:HG23	1:8:A:TYR:HB3	4	0.29
(1,376)	1:8:A:TYR:HA	1:24:A:PRO:HD3	2	0.29
(1,327)	1:8:A:TYR:HB3	1:9:A:ILE:H	3	0.29
(1,283)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	1	0.29
(1,263)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	9	0.29
(1,225)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	7	0.29
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	3	0.29
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	3	0.29
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	5	0.29
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	5	0.29
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	8	0.29
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	8	0.29
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	9	0.29
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	9	0.29
(1,188)	1:14:A:GLN:H	1:14:A:GLN:HG3	4	0.29
(1,178)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	7	0.29
(1,178)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	7	0.29
(1,178)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	7	0.29
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	10	0.29
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	10	0.29
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	10	0.29
(1,96)	1:8:A:TYR:HA	1:8:A:TYR:HB2	2	0.29
(1,96)	1:8:A:TYR:HA	1:8:A:TYR:HB2	4	0.29
(1,96)	1:8:A:TYR:HA	1:8:A:TYR:HB2	9	0.29
(1,85)	1:7:A:LEU:HD11	1:7:A:LEU:HG	5	0.29
(1,85)	1:7:A:LEU:HD12	1:7:A:LEU:HG	5	0.29
(1,85)	1:7:A:LEU:HD13	1:7:A:LEU:HG	5	0.29
(1,85)	1:7:A:LEU:HD11	1:7:A:LEU:HG	6	0.29
(1,85)	1:7:A:LEU:HD12	1:7:A:LEU:HG	6	0.29
(1,85)	1:7:A:LEU:HD13	1:7:A:LEU:HG	6	0.29
(1,85)	1:7:A:LEU:HD11	1:7:A:LEU:HG	9	0.29
(1,85)	1:7:A:LEU:HD12	1:7:A:LEU:HG	9	0.29
(1,85)	1:7:A:LEU:HD13	1:7:A:LEU:HG	9	0.29
(1,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	8	0.29
(4,31)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	2	0.28
(4,28)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	9	0.28
(4,28)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	9	0.28
(4,28)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	9	0.28
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	8	0.28
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	8	0.28
(4,24)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	8	0.28
(4,13)	1:11:A:TRP:H	1:11:A:TRP:HD1	6	0.28
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG2	1	0.28
(4,1)	1:3:A:GLU:H	1:3:A:GLU:HG3	1	0.28
(3,360)	1:15:A:GLY:HA3	1:18:A:SER:HB3	4	0.28
(3,176)	1:14:A:GLN:HA	1:14:A:GLN:HG2	5	0.28
(3,114)	1:10:A:GLN:H	1:10:A:GLN:HB2	4	0.28
(2,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	2	0.28
(2,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	9	0.28
(2,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	9	0.28
(2,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	9	0.28
(2,386)	1:15:A:GLY:HA3	1:18:A:SER:HB3	4	0.28
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	8	0.28
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	8	0.28
(2,364)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	8	0.28
(2,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	5	0.28
(2,139)	1:11:A:TRP:H	1:11:A:TRP:HD1	6	0.28
(2,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG2	1	0.28
(2,21)	1:3:A:GLU:H	1:3:A:GLU:HG3	1	0.28
(1,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	4	0.28
(1,435)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	10	0.28
(1,435)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	10	0.28
(1,435)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	10	0.28
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	9	0.28
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	9	0.28
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	9	0.28
(1,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	10	0.28
(1,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	6	0.28
(1,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	6	0.28
(1,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	6	0.28
(1,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	9	0.28
(1,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	9	0.28
(1,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	9	0.28
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	6	0.28
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	6	0.28
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	6	0.28
(1,376)	1:8:A:TYR:HA	1:24:A:PRO:HD3	4	0.28
(1,314)	1:8:A:TYR:HD1	1:9:A:ILE:H	8	0.28
(1,314)	1:8:A:TYR:HD2	1:9:A:ILE:H	8	0.28
(1,283)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	4	0.28
(1,267)	1:24:A:PRO:HA	1:24:A:PRO:HB3	3	0.28
(1,267)	1:24:A:PRO:HA	1:24:A:PRO:HB3	8	0.28
(1,263)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	3	0.28
(1,225)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	3	0.28
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.28
(1,210)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	10	0.28
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG2	7	0.28
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG3	7	0.28
(1,198)	1:19:A:SER:H	1:19:A:SER:HB3	4	0.28
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	8	0.28
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	8	0.28
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	8	0.28
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB2	8	0.28
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB3	8	0.28
(1,96)	1:8:A:TYR:HA	1:8:A:TYR:HB2	5	0.28
(1,96)	1:8:A:TYR:HA	1:8:A:TYR:HB2	7	0.28
(1,96)	1:8:A:TYR:HA	1:8:A:TYR:HB2	8	0.28
(1,85)	1:7:A:LEU:HD11	1:7:A:LEU:HG	1	0.28
(1,85)	1:7:A:LEU:HD12	1:7:A:LEU:HG	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:7:A:LEU:HD13	1:7:A:LEU:HG	1	0.28
(1,81)	1:7:A:LEU:HB3	1:7:A:LEU:HG	10	0.28
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	2	0.28
(1,56)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	4	0.28
(1,52)	1:6:A:ARG:HA	1:6:A:ARG:HG2	9	0.28
(1,26)	1:3:A:GLU:HG2	1:4:A:ALA:H	2	0.28
(1,26)	1:3:A:GLU:HG3	1:4:A:ALA:H	2	0.28
(1,26)	1:3:A:GLU:HG2	1:4:A:ALA:H	9	0.28
(1,26)	1:3:A:GLU:HG3	1:4:A:ALA:H	9	0.28
(4,40)	1:3:A:GLU:HG2	1:6:A:ARG:H	7	0.27
(4,40)	1:3:A:GLU:HG3	1:6:A:ARG:H	7	0.27
(4,31)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	4	0.27
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	2	0.27
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	2	0.27
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	2	0.27
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	4	0.27
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	4	0.27
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	4	0.27
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	6	0.27
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	6	0.27
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	6	0.27
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.27
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.27
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.27
(4,3)	1:6:A:ARG:HA	1:6:A:ARG:HD2	1	0.27
(4,3)	1:6:A:ARG:HA	1:6:A:ARG:HD2	7	0.27
(3,114)	1:10:A:GLN:H	1:10:A:GLN:HB2	3	0.27
(2,461)	1:3:A:GLU:HG2	1:6:A:ARG:H	7	0.27
(2,461)	1:3:A:GLU:HG3	1:6:A:ARG:H	7	0.27
(2,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	4	0.27
(2,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	3	0.27
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD11	2	0.27
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD12	2	0.27
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD13	2	0.27
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD11	4	0.27
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD12	4	0.27
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD13	4	0.27
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD11	6	0.27
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD12	6	0.27
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD13	6	0.27
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.27
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.27
(2,48)	1:6:A:ARG:HA	1:6:A:ARG:HD2	1	0.27
(2,48)	1:6:A:ARG:HA	1:6:A:ARG:HD2	7	0.27
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	5	0.27
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	5	0.27
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	5	0.27
(1,419)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	1	0.27
(1,419)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	3	0.27
(1,419)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	4	0.27
(1,419)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	5	0.27
(1,419)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	6	0.27
(1,419)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	8	0.27
(1,419)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	9	0.27
(1,419)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	10	0.27
(1,370)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	8	0.27
(1,370)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	8	0.27
(1,370)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	8	0.27
(1,370)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	8	0.27
(1,370)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	8	0.27
(1,370)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	8	0.27
(1,370)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	8	0.27
(1,370)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	8	0.27
(1,370)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	8	0.27
(1,370)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	8	0.27
(1,370)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	8	0.27
(1,370)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	8	0.27
(1,271)	1:20:A:GLY:H	1:20:A:GLY:HA2	1	0.27
(1,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	1	0.27
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG2	10	0.27
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG3	10	0.27
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	3	0.27
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	3	0.27
(1,169)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	3	0.27
(1,155)	1:12:A:LEU:HA	1:16:A:GLY:H	5	0.27
(1,150)	1:15:A:GLY:HA2	1:16:A:GLY:H	1	0.27
(1,150)	1:15:A:GLY:HA2	1:16:A:GLY:H	4	0.27
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	2	0.27
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB3	2	0.27
(1,99)	1:8:A:TYR:H	1:8:A:TYR:HB3	7	0.27
(1,81)	1:7:A:LEU:HB3	1:7:A:LEU:HG	3	0.27
(1,81)	1:7:A:LEU:HB3	1:7:A:LEU:HG	9	0.27
(1,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	4	0.27
(1,51)	1:6:A:ARG:HA	1:6:A:ARG:HB3	7	0.27
(4,40)	1:3:A:GLU:HG2	1:6:A:ARG:H	2	0.26
(4,40)	1:3:A:GLU:HG3	1:6:A:ARG:H	2	0.26
(4,40)	1:3:A:GLU:HG2	1:6:A:ARG:H	6	0.26
(4,40)	1:3:A:GLU:HG3	1:6:A:ARG:H	6	0.26
(4,40)	1:3:A:GLU:HG2	1:6:A:ARG:H	9	0.26
(4,40)	1:3:A:GLU:HG3	1:6:A:ARG:H	9	0.26
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	5	0.26
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	5	0.26
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	5	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.26
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.26
(4,3)	1:6:A:ARG:HA	1:6:A:ARG:HD2	3	0.26
(3,361)	1:5:A:VAL:HA	1:8:A:TYR:HB2	8	0.26
(3,300)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	10	0.26
(3,176)	1:14:A:GLN:HA	1:14:A:GLN:HG2	4	0.26
(3,176)	1:14:A:GLN:HA	1:14:A:GLN:HG2	9	0.26
(3,65)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.26
(3,46)	1:6:A:ARG:HA	1:6:A:ARG:HD3	6	0.26
(2,461)	1:3:A:GLU:HG2	1:6:A:ARG:H	2	0.26
(2,461)	1:3:A:GLU:HG3	1:6:A:ARG:H	2	0.26
(2,461)	1:3:A:GLU:HG2	1:6:A:ARG:H	6	0.26
(2,461)	1:3:A:GLU:HG3	1:6:A:ARG:H	6	0.26
(2,461)	1:3:A:GLU:HG2	1:6:A:ARG:H	9	0.26
(2,461)	1:3:A:GLU:HG3	1:6:A:ARG:H	9	0.26
(2,387)	1:5:A:VAL:HA	1:8:A:TYR:HB2	8	0.26
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	10	0.26
(2,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	4	0.26
(2,190)	1:14:A:GLN:HA	1:14:A:GLN:HG2	9	0.26
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD11	5	0.26
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD12	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD13	5	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.26
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.26
(2,68)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.26
(2,49)	1:6:A:ARG:HA	1:6:A:ARG:HD3	6	0.26
(2,48)	1:6:A:ARG:HA	1:6:A:ARG:HD2	3	0.26
(1,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	1	0.26
(1,431)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	2	0.26
(1,431)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	2	0.26
(1,431)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	2	0.26
(1,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	9	0.26
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	4	0.26
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	4	0.26
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	4	0.26
(1,419)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	2	0.26
(1,419)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	7	0.26
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD21	10	0.26
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD22	10	0.26
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD23	10	0.26
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	8	0.26
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	8	0.26
(1,285)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	1	0.26
(1,285)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	2	0.26
(1,285)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	3	0.26
(1,285)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	4	0.26
(1,285)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	6	0.26
(1,285)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	7	0.26
(1,285)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	8	0.26
(1,285)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	10	0.26
(1,273)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	1	0.26
(1,273)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	9	0.26
(1,267)	1:24:A:PRO:HA	1:24:A:PRO:HB3	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:24:A:PRO:HA	1:24:A:PRO:HB3	2	0.26
(1,267)	1:24:A:PRO:HA	1:24:A:PRO:HB3	4	0.26
(1,263)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	10	0.26
(1,241)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	1	0.26
(1,241)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	2	0.26
(1,241)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	4	0.26
(1,241)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	6	0.26
(1,241)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	8	0.26
(1,241)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.26
(1,225)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	2	0.26
(1,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	9	0.26
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	4	0.26
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB3	4	0.26
(1,99)	1:8:A:TYR:H	1:8:A:TYR:HB3	10	0.26
(1,96)	1:8:A:TYR:HA	1:8:A:TYR:HB2	1	0.26
(1,81)	1:7:A:LEU:HB3	1:7:A:LEU:HG	2	0.26
(1,81)	1:7:A:LEU:HB3	1:7:A:LEU:HG	4	0.26
(1,81)	1:7:A:LEU:HB3	1:7:A:LEU:HG	6	0.26
(1,81)	1:7:A:LEU:HB3	1:7:A:LEU:HG	8	0.26
(1,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	9	0.26
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	8	0.26
(1,30)	1:4:A:ALA:HA	1:5:A:VAL:H	3	0.26
(1,30)	1:4:A:ALA:HA	1:5:A:VAL:H	9	0.26
(1,25)	1:3:A:GLU:HG2	1:4:A:ALA:HA	2	0.26
(1,25)	1:3:A:GLU:HG3	1:4:A:ALA:HA	2	0.26
(4,40)	1:3:A:GLU:HG2	1:6:A:ARG:H	5	0.25
(4,40)	1:3:A:GLU:HG3	1:6:A:ARG:H	5	0.25
(4,17)	1:22:A:PRO:HA	1:22:A:PRO:HD3	8	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	1	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	1	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	1	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	3	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	3	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	3	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	9	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	9	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	9	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	10	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	10	0.25
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	10	0.25
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.25
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.25
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.25
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.25
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.25
(4,3)	1:6:A:ARG:HA	1:6:A:ARG:HD2	4	0.25
(4,3)	1:6:A:ARG:HA	1:6:A:ARG:HD2	10	0.25
(3,381)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	8	0.25
(3,370)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	9	0.25
(3,370)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	9	0.25
(3,370)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	9	0.25
(3,327)	1:24:A:PRO:HB3	1:25:A:SER:H	1	0.25
(3,327)	1:24:A:PRO:HB3	1:25:A:SER:H	2	0.25
(3,65)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.25
(3,65)	1:6:A:ARG:H	1:6:A:ARG:HB2	6	0.25
(2,461)	1:3:A:GLU:HG2	1:6:A:ARG:H	5	0.25
(2,461)	1:3:A:GLU:HG3	1:6:A:ARG:H	5	0.25
(2,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	8	0.25
(2,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	9	0.25
(2,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	9	0.25
(2,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	9	0.25
(2,349)	1:24:A:PRO:HB3	1:25:A:SER:H	1	0.25
(2,349)	1:24:A:PRO:HB3	1:25:A:SER:H	2	0.25
(2,215)	1:22:A:PRO:HA	1:22:A:PRO:HD3	8	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD11	1	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD12	1	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD13	1	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD11	3	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD12	3	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD13	3	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD11	9	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD12	9	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD13	9	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD11	10	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD12	10	0.25
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD13	10	0.25
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.25
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.25
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.25
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.25
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.25
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.25
(2,68)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:6:A:ARG:H	1:6:A:ARG:HB2	6	0.25
(2,48)	1:6:A:ARG:HA	1:6:A:ARG:HD2	4	0.25
(2,48)	1:6:A:ARG:HA	1:6:A:ARG:HD2	10	0.25
(1,472)	1:13:A:LYS:H	1:14:A:GLN:HA	10	0.25
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	7	0.25
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	7	0.25
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	7	0.25
(1,420)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	3	0.25
(1,420)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	3	0.25
(1,417)	1:8:A:TYR:HB3	1:24:A:PRO:HD2	10	0.25
(1,416)	1:8:A:TYR:HB2	1:24:A:PRO:HD2	9	0.25
(1,399)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	5	0.25
(1,399)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	5	0.25
(1,399)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	5	0.25
(1,399)	1:5:A:VAL:HG21	1:8:A:TYR:HB3	5	0.25
(1,399)	1:5:A:VAL:HG22	1:8:A:TYR:HB3	5	0.25
(1,399)	1:5:A:VAL:HG23	1:8:A:TYR:HB3	5	0.25
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	3	0.25
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	3	0.25
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	5	0.25
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	5	0.25
(1,285)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	5	0.25
(1,285)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	9	0.25
(1,279)	1:21:A:ARG:HA	1:21:A:ARG:HG2	10	0.25
(1,273)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	2	0.25
(1,273)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	3	0.25
(1,273)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	4	0.25
(1,273)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	5	0.25
(1,273)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	6	0.25
(1,273)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	7	0.25
(1,273)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	8	0.25
(1,273)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	10	0.25
(1,267)	1:24:A:PRO:HA	1:24:A:PRO:HB3	10	0.25
(1,252)	1:23:A:PRO:HA	1:24:A:PRO:HD3	3	0.25
(1,241)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	5	0.25
(1,241)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	7	0.25
(1,241)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	9	0.25
(1,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.25
(1,174)	1:13:A:LYS:HA	1:13:A:LYS:HB2	10	0.25
(1,174)	1:13:A:LYS:HA	1:13:A:LYS:HB3	10	0.25
(1,133)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	7	0.25
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB3	1	0.25
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	3	0.25
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB3	3	0.25
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	5	0.25
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB3	5	0.25
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	9	0.25
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB3	9	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB2	1	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB3	1	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB2	2	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB3	2	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB2	4	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB3	4	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB2	5	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB3	5	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB2	6	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB3	6	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB2	9	0.25
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB3	9	0.25
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	5	0.25
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	5	0.25
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	5	0.25
(1,99)	1:8:A:TYR:H	1:8:A:TYR:HB3	3	0.25
(1,99)	1:8:A:TYR:H	1:8:A:TYR:HB3	4	0.25
(1,96)	1:8:A:TYR:HA	1:8:A:TYR:HB2	6	0.25
(1,81)	1:7:A:LEU:HB3	1:7:A:LEU:HG	1	0.25
(1,56)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	8	0.25
(1,31)	1:4:A:ALA:H	1:5:A:VAL:H	1	0.25
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	1	0.24
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	1	0.24
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	1	0.24
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	1	0.24
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	1	0.24
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	1	0.24
(4,40)	1:3:A:GLU:HG2	1:6:A:ARG:H	10	0.24
(4,40)	1:3:A:GLU:HG3	1:6:A:ARG:H	10	0.24
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG21	3	0.24
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG22	3	0.24
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG23	3	0.24
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG21	5	0.24
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG22	5	0.24
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG23	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG21	6	0.24
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG22	6	0.24
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG23	6	0.24
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.24
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.24
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.24
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD21	1	0.24
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD22	1	0.24
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD23	1	0.24
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD21	9	0.24
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD22	9	0.24
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD23	9	0.24
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	9	0.24
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	9	0.24
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	9	0.24
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	9	0.24
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	9	0.24
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	9	0.24
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	9	0.24
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	9	0.24
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	9	0.24
(3,381)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	7	0.24
(3,314)	1:7:A:LEU:HB3	1:8:A:TYR:H	3	0.24
(3,314)	1:7:A:LEU:HB3	1:8:A:TYR:H	10	0.24
(3,300)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	8	0.24
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	1	0.24
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	1	0.24
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	1	0.24
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	1	0.24
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	1	0.24
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	1	0.24
(2,461)	1:3:A:GLU:HG2	1:6:A:ARG:H	10	0.24
(2,461)	1:3:A:GLU:HG3	1:6:A:ARG:H	10	0.24
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	9	0.24
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	9	0.24
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	9	0.24
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	9	0.24
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	9	0.24
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	9	0.24
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	9	0.24
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	9	0.24
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,410)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	7	0.24
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG21	3	0.24
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG22	3	0.24
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG23	3	0.24
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG21	5	0.24
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG22	5	0.24
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG23	5	0.24
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG21	6	0.24
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG22	6	0.24
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG23	6	0.24
(2,335)	1:7:A:LEU:HB3	1:8:A:TYR:H	3	0.24
(2,335)	1:7:A:LEU:HB3	1:8:A:TYR:H	10	0.24
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	8	0.24
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.24
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.24
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.24
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD21	1	0.24
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD22	1	0.24
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD23	1	0.24
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD21	9	0.24
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD22	9	0.24
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD23	9	0.24
(1,472)	1:13:A:LYS:H	1:14:A:GLN:HA	8	0.24
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	10	0.24
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	10	0.24
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	10	0.24
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	2	0.24
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	2	0.24
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	2	0.24
(1,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB2	1	0.24
(1,424)	1:13:A:LYS:HB2	1:14:A:GLN:HB3	1	0.24
(1,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB2	1	0.24
(1,424)	1:13:A:LYS:HB3	1:14:A:GLN:HB3	1	0.24
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	5	0.24
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	5	0.24
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	5	0.24
(1,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	4	0.24
(1,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	4	0.24
(1,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	4	0.24
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD21	4	0.24
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD22	4	0.24
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD23	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD21	5	0.24
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD22	5	0.24
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD23	5	0.24
(1,361)	1:14:A:GLN:HE22	1:21:A:ARG:HG3	2	0.24
(1,319)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	7	0.24
(1,289)	1:15:A:GLY:H	1:16:A:GLY:H	1	0.24
(1,289)	1:15:A:GLY:H	1:16:A:GLY:H	2	0.24
(1,267)	1:24:A:PRO:HA	1:24:A:PRO:HB3	6	0.24
(1,241)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	3	0.24
(1,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	4	0.24
(1,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	5	0.24
(1,133)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	10	0.24
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB2	3	0.24
(1,125)	1:10:A:GLN:HA	1:10:A:GLN:HB3	3	0.24
(1,123)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	8	0.24
(1,99)	1:8:A:TYR:H	1:8:A:TYR:HB3	8	0.24
(1,84)	1:7:A:LEU:HD21	1:7:A:LEU:HG	1	0.24
(1,84)	1:7:A:LEU:HD22	1:7:A:LEU:HG	1	0.24
(1,84)	1:7:A:LEU:HD23	1:7:A:LEU:HG	1	0.24
(1,84)	1:7:A:LEU:HD21	1:7:A:LEU:HG	4	0.24
(1,84)	1:7:A:LEU:HD22	1:7:A:LEU:HG	4	0.24
(1,84)	1:7:A:LEU:HD23	1:7:A:LEU:HG	4	0.24
(1,84)	1:7:A:LEU:HD21	1:7:A:LEU:HG	7	0.24
(1,84)	1:7:A:LEU:HD22	1:7:A:LEU:HG	7	0.24
(1,84)	1:7:A:LEU:HD23	1:7:A:LEU:HG	7	0.24
(1,81)	1:7:A:LEU:HB3	1:7:A:LEU:HG	5	0.24
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	1	0.24
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	6	0.24
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	7	0.24
(1,56)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	2	0.24
(1,51)	1:6:A:ARG:HA	1:6:A:ARG:HB3	5	0.24
(1,51)	1:6:A:ARG:HA	1:6:A:ARG:HB3	6	0.24
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG11	7	0.24
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG12	7	0.24
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG13	7	0.24
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG21	7	0.24
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG22	7	0.24
(1,38)	1:4:A:ALA:H	1:5:A:VAL:HG23	7	0.24
(1,30)	1:4:A:ALA:HA	1:5:A:VAL:H	2	0.24
(1,25)	1:3:A:GLU:HG2	1:4:A:ALA:HA	9	0.24
(1,25)	1:3:A:GLU:HG3	1:4:A:ALA:HA	9	0.24
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	4	0.23
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	4	0.23
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	4	0.23
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	4	0.23
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	4	0.23
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD21	2	0.23
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD22	2	0.23
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD23	2	0.23
(4,3)	1:6:A:ARG:HA	1:6:A:ARG:HD2	8	0.23
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG11	7	0.23
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG12	7	0.23
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG13	7	0.23
(3,314)	1:7:A:LEU:HB3	1:8:A:TYR:H	2	0.23
(3,70)	1:6:A:ARG:HB2	1:7:A:LEU:H	6	0.23
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	4	0.23
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	4	0.23
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	4	0.23
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	4	0.23
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	4	0.23
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	4	0.23
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG11	7	0.23
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG12	7	0.23
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG13	7	0.23
(2,335)	1:7:A:LEU:HB3	1:8:A:TYR:H	2	0.23
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD21	2	0.23
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD22	2	0.23
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD23	2	0.23
(2,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	6	0.23
(2,48)	1:6:A:ARG:HA	1:6:A:ARG:HD2	8	0.23
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	7	0.23
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB3	7	0.23
(1,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	6	0.23
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	4	0.23
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	4	0.23
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	4	0.23
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	4	0.23
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	4	0.23
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	4	0.23
(1,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	4	0.23
(1,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	4	0.23
(1,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	4	0.23
(1,420)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	5	0.23
(1,420)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	9	0.23
(1,420)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	9	0.23
(1,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	1	0.23
(1,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	1	0.23
(1,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	1	0.23
(1,399)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	2	0.23
(1,399)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	2	0.23
(1,399)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	2	0.23
(1,399)	1:5:A:VAL:HG21	1:8:A:TYR:HB3	2	0.23
(1,399)	1:5:A:VAL:HG22	1:8:A:TYR:HB3	2	0.23
(1,399)	1:5:A:VAL:HG23	1:8:A:TYR:HB3	2	0.23
(1,346)	1:14:A:GLN:HE21	1:14:A:GLN:HG2	8	0.23
(1,341)	1:21:A:ARG:H	1:21:A:ARG:HG2	10	0.23
(1,316)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	8	0.23
(1,316)	1:11:A:TRP:HE1	1:23:A:PRO:HD3	8	0.23
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG2	3	0.23
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG3	3	0.23
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG2	8	0.23
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG3	8	0.23
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	2	0.23
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	2	0.23
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	2	0.23
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	2	0.23
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	4	0.23
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	4	0.23
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	4	0.23
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	4	0.23
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	6	0.23
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	6	0.23
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	6	0.23
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	6	0.23
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	10	0.23
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	10	0.23
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	10	0.23
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	10	0.23
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE2	3	0.23
(1,171)	1:13:A:LYS:HA	1:13:A:LYS:HE3	3	0.23
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	6	0.23
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB3	6	0.23
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	7	0.23
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB3	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	10	0.23
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB3	10	0.23
(1,123)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	7	0.23
(1,123)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	10	0.23
(1,99)	1:8:A:TYR:H	1:8:A:TYR:HB3	5	0.23
(1,84)	1:7:A:LEU:HD21	1:7:A:LEU:HG	2	0.23
(1,84)	1:7:A:LEU:HD22	1:7:A:LEU:HG	2	0.23
(1,84)	1:7:A:LEU:HD23	1:7:A:LEU:HG	2	0.23
(1,84)	1:7:A:LEU:HD21	1:7:A:LEU:HG	3	0.23
(1,84)	1:7:A:LEU:HD22	1:7:A:LEU:HG	3	0.23
(1,84)	1:7:A:LEU:HD23	1:7:A:LEU:HG	3	0.23
(1,30)	1:4:A:ALA:HA	1:5:A:VAL:H	4	0.23
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG21	10	0.22
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG22	10	0.22
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG23	10	0.22
(4,17)	1:22:A:PRO:HA	1:22:A:PRO:HD3	5	0.22
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD21	4	0.22
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD22	4	0.22
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD23	4	0.22
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD21	6	0.22
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD22	6	0.22
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD23	6	0.22
(3,424)	1:3:A:GLU:HA	1:6:A:ARG:HB2	1	0.22
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	3	0.22
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	3	0.22
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	3	0.22
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	3	0.22
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	3	0.22
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	3	0.22
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	3	0.22
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	3	0.22
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	3	0.22
(3,382)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	9	0.22
(3,300)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	4	0.22
(3,70)	1:6:A:ARG:HB2	1:7:A:LEU:H	7	0.22
(2,464)	1:3:A:GLU:HA	1:6:A:ARG:HB2	1	0.22
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	3	0.22
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	3	0.22
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	3	0.22
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	3	0.22
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	3	0.22
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	3	0.22
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	3	0.22
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	3	0.22
(2,411)	1:6:A:ARG:HD3	1:7:A:LEU:HB2	9	0.22
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG21	10	0.22
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG22	10	0.22
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG23	10	0.22
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	4	0.22
(2,215)	1:22:A:PRO:HA	1:22:A:PRO:HD3	5	0.22
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD21	4	0.22
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD22	4	0.22
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD23	4	0.22
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD21	6	0.22
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD22	6	0.22
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD23	6	0.22
(2,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	7	0.22
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB1	7	0.22
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB2	7	0.22
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB3	7	0.22
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG11	7	0.22
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG12	7	0.22
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG13	7	0.22
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG21	7	0.22
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG22	7	0.22
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG23	7	0.22
(1,414)	1:12:A:LEU:HA	1:17:A:PRO:HD2	6	0.22
(1,399)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	7	0.22
(1,399)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	7	0.22
(1,399)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	7	0.22
(1,399)	1:5:A:VAL:HG21	1:8:A:TYR:HB3	7	0.22
(1,399)	1:5:A:VAL:HG22	1:8:A:TYR:HB3	7	0.22
(1,399)	1:5:A:VAL:HG23	1:8:A:TYR:HB3	7	0.22
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD21	1	0.22
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD22	1	0.22
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD23	1	0.22
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD21	2	0.22
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD22	2	0.22
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD23	2	0.22
(1,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	6	0.22
(1,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	6	0.22
(1,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	6	0.22
(1,381)	1:6:A:ARG:HA	1:9:A:ILE:HB	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,380)	1:8:A:TYR:HA	1:24:A:PRO:HG3	9	0.22
(1,314)	1:8:A:TYR:HD1	1:9:A:ILE:H	1	0.22
(1,314)	1:8:A:TYR:HD2	1:9:A:ILE:H	1	0.22
(1,282)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	5	0.22
(1,271)	1:20:A:GLY:H	1:20:A:GLY:HA2	6	0.22
(1,250)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	1	0.22
(1,250)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	4	0.22
(1,250)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	7	0.22
(1,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	2	0.22
(1,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	3	0.22
(1,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	6	0.22
(1,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	7	0.22
(1,214)	1:22:A:PRO:HA	1:22:A:PRO:HD2	8	0.22
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	2	0.22
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	2	0.22
(1,198)	1:19:A:SER:H	1:19:A:SER:HB3	6	0.22
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	1	0.22
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	1	0.22
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	1	0.22
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	1	0.22
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	3	0.22
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	3	0.22
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	3	0.22
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	3	0.22
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	5	0.22
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	5	0.22
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	5	0.22
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	5	0.22
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	9	0.22
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	9	0.22
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	9	0.22
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	9	0.22
(1,156)	1:12:A:LEU:HA	1:12:A:LEU:HB2	4	0.22
(1,123)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	1	0.22
(1,123)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	2	0.22
(1,123)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	3	0.22
(1,123)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	4	0.22
(1,123)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	5	0.22
(1,123)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	6	0.22
(1,123)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	9	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	1	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	1	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	2	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	2	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	2	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	7	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	7	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	7	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	8	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	8	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	8	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	9	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	9	0.22
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	9	0.22
(1,99)	1:8:A:TYR:H	1:8:A:TYR:HB3	1	0.22
(1,99)	1:8:A:TYR:H	1:8:A:TYR:HB3	2	0.22
(1,99)	1:8:A:TYR:H	1:8:A:TYR:HB3	9	0.22
(1,84)	1:7:A:LEU:HD21	1:7:A:LEU:HG	5	0.22
(1,84)	1:7:A:LEU:HD22	1:7:A:LEU:HG	5	0.22
(1,84)	1:7:A:LEU:HD23	1:7:A:LEU:HG	5	0.22
(1,84)	1:7:A:LEU:HD21	1:7:A:LEU:HG	6	0.22
(1,84)	1:7:A:LEU:HD22	1:7:A:LEU:HG	6	0.22
(1,84)	1:7:A:LEU:HD23	1:7:A:LEU:HG	6	0.22
(1,84)	1:7:A:LEU:HD21	1:7:A:LEU:HG	8	0.22
(1,84)	1:7:A:LEU:HD22	1:7:A:LEU:HG	8	0.22
(1,84)	1:7:A:LEU:HD23	1:7:A:LEU:HG	8	0.22
(1,84)	1:7:A:LEU:HD21	1:7:A:LEU:HG	9	0.22
(1,84)	1:7:A:LEU:HD22	1:7:A:LEU:HG	9	0.22
(1,84)	1:7:A:LEU:HD23	1:7:A:LEU:HG	9	0.22
(1,84)	1:7:A:LEU:HD21	1:7:A:LEU:HG	10	0.22
(1,84)	1:7:A:LEU:HD22	1:7:A:LEU:HG	10	0.22
(1,84)	1:7:A:LEU:HD23	1:7:A:LEU:HG	10	0.22
(1,81)	1:7:A:LEU:HB3	1:7:A:LEU:HG	7	0.22
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	0.22
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	0.22
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	0.22
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	5	0.22
(1,56)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	10	0.22
(1,30)	1:4:A:ALA:HA	1:5:A:VAL:H	5	0.22
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	2	0.21
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	2	0.21
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	2	0.21
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	2	0.21
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	2	0.21
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	7	0.21
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	7	0.21
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	7	0.21
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	7	0.21
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	7	0.21
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	7	0.21
(4,17)	1:22:A:PRO:HA	1:22:A:PRO:HD3	10	0.21
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.21
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.21
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.21
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.21
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.21
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.21
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD21	8	0.21
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD22	8	0.21
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD23	8	0.21
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD21	10	0.21
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD22	10	0.21
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD23	10	0.21
(4,3)	1:6:A:ARG:HA	1:6:A:ARG:HD2	2	0.21
(4,2)	1:4:A:ALA:H	1:5:A:VAL:HB	1	0.21
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	2	0.21
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	2	0.21
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	2	0.21
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	2	0.21
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	2	0.21
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	2	0.21
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	2	0.21
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	2	0.21
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	2	0.21
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	5	0.21
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	5	0.21
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	5	0.21
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	5	0.21
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	5	0.21
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	5	0.21
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	5	0.21
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	5	0.21
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	5	0.21
(3,314)	1:7:A:LEU:HB3	1:8:A:TYR:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,314)	1:7:A:LEU:HB3	1:8:A:TYR:H	6	0.21
(3,314)	1:7:A:LEU:HB3	1:8:A:TYR:H	8	0.21
(3,314)	1:7:A:LEU:HB3	1:8:A:TYR:H	9	0.21
(3,118)	1:10:A:GLN:H	1:10:A:GLN:HG3	7	0.21
(3,70)	1:6:A:ARG:HB2	1:7:A:LEU:H	5	0.21
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	2	0.21
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	2	0.21
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	2	0.21
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	2	0.21
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	2	0.21
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	2	0.21
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	7	0.21
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	7	0.21
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	7	0.21
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	7	0.21
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	7	0.21
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	7	0.21
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	2	0.21
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	2	0.21
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	2	0.21
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	2	0.21
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	2	0.21
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	2	0.21
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	2	0.21
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	2	0.21
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	2	0.21
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	5	0.21
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	5	0.21
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	5	0.21
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	5	0.21
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	5	0.21
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	5	0.21
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	5	0.21
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	5	0.21
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	5	0.21
(2,335)	1:7:A:LEU:HB3	1:8:A:TYR:H	4	0.21
(2,335)	1:7:A:LEU:HB3	1:8:A:TYR:H	6	0.21
(2,335)	1:7:A:LEU:HB3	1:8:A:TYR:H	8	0.21
(2,335)	1:7:A:LEU:HB3	1:8:A:TYR:H	9	0.21
(2,215)	1:22:A:PRO:HA	1:22:A:PRO:HD3	10	0.21
(2,130)	1:10:A:GLN:H	1:10:A:GLN:HG3	7	0.21
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.21
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.21
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.21
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.21
(2,118)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.21
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD21	8	0.21
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD22	8	0.21
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD23	8	0.21
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD21	10	0.21
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD22	10	0.21
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD23	10	0.21
(2,74)	1:6:A:ARG:HB2	1:7:A:LEU:H	5	0.21
(2,48)	1:6:A:ARG:HA	1:6:A:ARG:HD2	2	0.21
(2,39)	1:4:A:ALA:H	1:5:A:VAL:HB	1	0.21
(1,447)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	7	0.21
(1,447)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	7	0.21
(1,447)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	7	0.21
(1,447)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	7	0.21
(1,447)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	7	0.21
(1,447)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	7	0.21
(1,447)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	7	0.21
(1,447)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	7	0.21
(1,447)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	7	0.21
(1,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	7	0.21
(1,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	7	0.21
(1,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	7	0.21
(1,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	7	0.21
(1,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	7	0.21
(1,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	7	0.21
(1,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	7	0.21
(1,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	7	0.21
(1,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	7	0.21
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	1	0.21
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	1	0.21
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	1	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG11	2	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG12	2	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG13	2	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG21	2	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG22	2	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG23	2	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG11	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG12	3	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG13	3	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG21	3	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG22	3	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG23	3	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG11	4	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG12	4	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG13	4	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG21	4	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG22	4	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG23	4	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG11	5	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG12	5	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG13	5	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG21	5	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG22	5	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG23	5	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG11	6	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG12	6	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG13	6	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG21	6	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG22	6	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG23	6	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG11	8	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG12	8	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG13	8	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG21	8	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG22	8	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG23	8	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG11	9	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG12	9	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG13	9	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG21	9	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG22	9	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG23	9	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG11	10	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG12	10	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG13	10	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG21	10	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG22	10	0.21
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG23	10	0.21
(1,427)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	8	0.21
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	8	0.21
(1,426)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	8	0.21
(1,420)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	4	0.21
(1,420)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	4	0.21
(1,416)	1:8:A:TYR:HB2	1:24:A:PRO:HD2	4	0.21
(1,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	3	0.21
(1,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	3	0.21
(1,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	3	0.21
(1,381)	1:6:A:ARG:HA	1:9:A:ILE:HB	5	0.21
(1,354)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	8	0.21
(1,288)	1:13:A:LYS:H	1:14:A:GLN:H	9	0.21
(1,275)	1:21:A:ARG:HA	1:22:A:PRO:HD3	8	0.21
(1,252)	1:23:A:PRO:HA	1:24:A:PRO:HD3	5	0.21
(1,250)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	2	0.21
(1,250)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	3	0.21
(1,250)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	5	0.21
(1,250)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	9	0.21
(1,250)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	10	0.21
(1,221)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	6	0.21
(1,195)	1:19:A:SER:HB2	1:19:A:SER:HB3	9	0.21
(1,195)	1:19:A:SER:HB2	1:19:A:SER:HB3	10	0.21
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	8	0.21
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	8	0.21
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	8	0.21
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	8	0.21
(1,156)	1:12:A:LEU:HA	1:12:A:LEU:HB2	1	0.21
(1,156)	1:12:A:LEU:HA	1:12:A:LEU:HB2	2	0.21
(1,144)	1:11:A:TRP:H	1:11:A:TRP:HB2	6	0.21
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	3	0.21
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	3	0.21
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	3	0.21
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	4	0.21
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	4	0.21
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	4	0.21
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.21
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.21
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.21
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.21
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.21
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.21
(1,72)	1:6:A:ARG:HD3	1:7:A:LEU:H	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	10	0.21
(1,30)	1:4:A:ALA:HA	1:5:A:VAL:H	6	0.21
(1,7)	1:19:A:SER:H	1:19:A:SER:HA	4	0.21
(4,17)	1:22:A:PRO:HA	1:22:A:PRO:HD3	4	0.2
(4,17)	1:22:A:PRO:HA	1:22:A:PRO:HD3	9	0.2
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD21	3	0.2
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD22	3	0.2
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD23	3	0.2
(4,3)	1:6:A:ARG:HA	1:6:A:ARG:HD2	6	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	4	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	4	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	4	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	4	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	4	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	4	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	4	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	4	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	4	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	7	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	7	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	7	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	7	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	7	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	7	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	7	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	7	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	7	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.2
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.2
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.2
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.2
(3,361)	1:5:A:VAL:HA	1:8:A:TYR:HB2	10	0.2
(3,345)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	2	0.2
(3,345)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	2	0.2
(3,345)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	2	0.2
(3,345)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	2	0.2
(3,345)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,345)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	2	0.2
(3,345)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	2	0.2
(3,345)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	2	0.2
(3,345)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	2	0.2
(3,345)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	2	0.2
(3,345)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	2	0.2
(3,345)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	2	0.2
(3,331)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	6	0.2
(3,327)	1:24:A:PRO:HB3	1:25:A:SER:H	4	0.2
(3,183)	1:19:A:SER:HA	1:19:A:SER:HB2	1	0.2
(3,35)	1:5:A:VAL:H	1:5:A:VAL:HB	2	0.2
(3,35)	1:5:A:VAL:H	1:5:A:VAL:HB	3	0.2
(3,35)	1:5:A:VAL:H	1:5:A:VAL:HB	5	0.2
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	4	0.2
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	4	0.2
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	4	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	4	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	4	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	4	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	4	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	4	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	4	0.2
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	7	0.2
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	7	0.2
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	7	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	7	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	7	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	7	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	7	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	7	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	7	0.2
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.2
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.2
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.2
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.2
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.2
(2,387)	1:5:A:VAL:HA	1:8:A:TYR:HB2	10	0.2
(2,369)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,369)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	2	0.2
(2,369)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	2	0.2
(2,369)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	2	0.2
(2,369)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	2	0.2
(2,369)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	2	0.2
(2,369)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	2	0.2
(2,369)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	2	0.2
(2,369)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	2	0.2
(2,369)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	2	0.2
(2,369)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	2	0.2
(2,369)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	2	0.2
(2,353)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	6	0.2
(2,349)	1:24:A:PRO:HB3	1:25:A:SER:H	4	0.2
(2,215)	1:22:A:PRO:HA	1:22:A:PRO:HD3	4	0.2
(2,215)	1:22:A:PRO:HA	1:22:A:PRO:HD3	9	0.2
(2,197)	1:19:A:SER:HA	1:19:A:SER:HB2	1	0.2
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD21	3	0.2
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD22	3	0.2
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD23	3	0.2
(2,48)	1:6:A:ARG:HA	1:6:A:ARG:HD2	6	0.2
(2,36)	1:5:A:VAL:H	1:5:A:VAL:HB	2	0.2
(2,36)	1:5:A:VAL:H	1:5:A:VAL:HB	3	0.2
(2,36)	1:5:A:VAL:H	1:5:A:VAL:HB	5	0.2
(1,473)	1:5:A:VAL:HA	1:8:A:TYR:HD1	10	0.2
(1,473)	1:5:A:VAL:HA	1:8:A:TYR:HD2	10	0.2
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	2	0.2
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	2	0.2
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	2	0.2
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	9	0.2
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	9	0.2
(1,445)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	9	0.2
(1,421)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	3	0.2
(1,421)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	3	0.2
(1,420)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	10	0.2
(1,420)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	10	0.2
(1,414)	1:12:A:LEU:HA	1:17:A:PRO:HD2	7	0.2
(1,384)	1:7:A:LEU:HD11	1:8:A:TYR:HA	2	0.2
(1,384)	1:7:A:LEU:HD12	1:8:A:TYR:HA	2	0.2
(1,384)	1:7:A:LEU:HD13	1:8:A:TYR:HA	2	0.2
(1,346)	1:14:A:GLN:HE21	1:14:A:GLN:HG2	3	0.2
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	9	0.2
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	9	0.2
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	9	0.2
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	9	0.2
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	9	0.2
(1,283)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	9	0.2
(1,271)	1:20:A:GLY:H	1:20:A:GLY:HA2	7	0.2
(1,250)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	6	0.2
(1,250)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	8	0.2
(1,236)	1:23:A:PRO:HA	1:23:A:PRO:HB2	9	0.2
(1,221)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	3	0.2
(1,221)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	7	0.2
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	1	0.2
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	1	0.2
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	4	0.2
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	4	0.2
(1,205)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	4	0.2
(1,205)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	5	0.2
(1,205)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	9	0.2
(1,195)	1:19:A:SER:HB2	1:19:A:SER:HB3	1	0.2
(1,195)	1:19:A:SER:HB2	1:19:A:SER:HB3	5	0.2
(1,195)	1:19:A:SER:HB2	1:19:A:SER:HB3	8	0.2
(1,156)	1:12:A:LEU:HA	1:12:A:LEU:HB2	5	0.2
(1,156)	1:12:A:LEU:HA	1:12:A:LEU:HB2	9	0.2
(1,150)	1:15:A:GLY:HA2	1:16:A:GLY:H	2	0.2
(1,144)	1:11:A:TRP:H	1:11:A:TRP:HB2	7	0.2
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG21	7	0.2
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG22	7	0.2
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG23	7	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.2
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.2
(1,30)	1:4:A:ALA:HA	1:5:A:VAL:H	8	0.2
(1,30)	1:4:A:ALA:HA	1:5:A:VAL:H	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:3:A:GLU:HG2	1:4:A:ALA:H	1	0.2
(1,26)	1:3:A:GLU:HG3	1:4:A:ALA:H	1	0.2
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD21	5	0.19
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD22	5	0.19
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD23	5	0.19
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	6	0.19
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	6	0.19
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	6	0.19
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	6	0.19
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	6	0.19
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	6	0.19
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	6	0.19
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	6	0.19
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	6	0.19
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	1	0.19
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	1	0.19
(3,373)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	1	0.19
(3,361)	1:5:A:VAL:HA	1:8:A:TYR:HB2	7	0.19
(3,314)	1:7:A:LEU:HB3	1:8:A:TYR:H	1	0.19
(3,314)	1:7:A:LEU:HB3	1:8:A:TYR:H	5	0.19
(3,264)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	10	0.19
(3,183)	1:19:A:SER:HA	1:19:A:SER:HB2	10	0.19
(3,118)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.19
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	8	0.19
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	8	0.19
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	8	0.19
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.19
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.19
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.19
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.19
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.19
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.19
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.19
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.19
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.19
(3,35)	1:5:A:VAL:H	1:5:A:VAL:HB	4	0.19
(3,35)	1:5:A:VAL:H	1:5:A:VAL:HB	6	0.19
(3,35)	1:5:A:VAL:H	1:5:A:VAL:HB	9	0.19
(3,35)	1:5:A:VAL:H	1:5:A:VAL:HB	10	0.19
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	6	0.19
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	6	0.19
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	6	0.19
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	6	0.19
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	6	0.19
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	6	0.19
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	6	0.19
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	6	0.19
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	1	0.19
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	1	0.19
(2,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	1	0.19
(2,387)	1:5:A:VAL:HA	1:8:A:TYR:HB2	7	0.19
(2,335)	1:7:A:LEU:HB3	1:8:A:TYR:H	1	0.19
(2,335)	1:7:A:LEU:HB3	1:8:A:TYR:H	5	0.19
(2,281)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	10	0.19
(2,197)	1:19:A:SER:HA	1:19:A:SER:HB2	10	0.19
(2,130)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.19
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	8	0.19
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	8	0.19
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	8	0.19
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD21	5	0.19
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD22	5	0.19
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD23	5	0.19
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.19
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.19
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.19
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.19
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.19
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.19
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.19
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.19
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.19
(2,36)	1:5:A:VAL:H	1:5:A:VAL:HB	4	0.19
(2,36)	1:5:A:VAL:H	1:5:A:VAL:HB	6	0.19
(2,36)	1:5:A:VAL:H	1:5:A:VAL:HB	9	0.19
(2,36)	1:5:A:VAL:H	1:5:A:VAL:HB	10	0.19
(1,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	10	0.19
(1,431)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	9	0.19
(1,431)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	9	0.19
(1,431)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	9	0.19
(1,420)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	2	0.19
(1,420)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	2	0.19
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	3	0.19
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	3	0.19
(1,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	2	0.19
(1,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	2	0.19
(1,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	2	0.19
(1,394)	1:12:A:LEU:HD11	1:17:A:PRO:HD3	7	0.19
(1,394)	1:12:A:LEU:HD12	1:17:A:PRO:HD3	7	0.19
(1,394)	1:12:A:LEU:HD13	1:17:A:PRO:HD3	7	0.19
(1,384)	1:7:A:LEU:HD11	1:8:A:TYR:HA	10	0.19
(1,384)	1:7:A:LEU:HD12	1:8:A:TYR:HA	10	0.19
(1,384)	1:7:A:LEU:HD13	1:8:A:TYR:HA	10	0.19
(1,377)	1:8:A:TYR:HA	1:11:A:TRP:HB3	3	0.19
(1,376)	1:8:A:TYR:HA	1:24:A:PRO:HD3	9	0.19
(1,361)	1:14:A:GLN:HE22	1:21:A:ARG:HG3	7	0.19
(1,353)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	8	0.19
(1,344)	1:14:A:GLN:HE21	1:14:A:GLN:HG3	7	0.19
(1,338)	1:21:A:ARG:H	1:21:A:ARG:HB2	7	0.19
(1,323)	1:14:A:GLN:HA	1:15:A:GLY:H	9	0.19
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	1	0.19
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	1	0.19
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	4	0.19
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	4	0.19
(1,289)	1:15:A:GLY:H	1:16:A:GLY:H	5	0.19
(1,260)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	10	0.19
(1,236)	1:23:A:PRO:HA	1:23:A:PRO:HB2	1	0.19
(1,236)	1:23:A:PRO:HA	1:23:A:PRO:HB2	2	0.19
(1,236)	1:23:A:PRO:HA	1:23:A:PRO:HB2	3	0.19
(1,236)	1:23:A:PRO:HA	1:23:A:PRO:HB2	4	0.19
(1,236)	1:23:A:PRO:HA	1:23:A:PRO:HB2	5	0.19
(1,236)	1:23:A:PRO:HA	1:23:A:PRO:HB2	7	0.19
(1,236)	1:23:A:PRO:HA	1:23:A:PRO:HB2	8	0.19
(1,236)	1:23:A:PRO:HA	1:23:A:PRO:HB2	10	0.19
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	8	0.19
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	8	0.19
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	9	0.19
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	9	0.19
(1,205)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	1	0.19
(1,205)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	2	0.19
(1,205)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	3	0.19
(1,205)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	6	0.19
(1,205)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	7	0.19
(1,205)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	8	0.19
(1,205)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	9	0.19
(1,198)	1:19:A:SER:H	1:19:A:SER:HB3	7	0.19
(1,195)	1:19:A:SER:HB2	1:19:A:SER:HB3	2	0.19
(1,195)	1:19:A:SER:HB2	1:19:A:SER:HB3	3	0.19
(1,195)	1:19:A:SER:HB2	1:19:A:SER:HB3	4	0.19
(1,195)	1:19:A:SER:HB2	1:19:A:SER:HB3	6	0.19
(1,195)	1:19:A:SER:HB2	1:19:A:SER:HB3	7	0.19
(1,188)	1:14:A:GLN:H	1:14:A:GLN:HG3	6	0.19
(1,185)	1:14:A:GLN:HA	1:14:A:GLN:HE21	1	0.19
(1,146)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	3	0.19
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	10	0.19
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	10	0.19
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	10	0.19
(1,99)	1:8:A:TYR:H	1:8:A:TYR:HB3	6	0.19
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.19
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.19
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.19
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	3	0.19
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	9	0.19
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	8	0.18
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	8	0.18
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	8	0.18
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	8	0.18
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	8	0.18
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	8	0.18
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG21	2	0.18
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG22	2	0.18
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG23	2	0.18
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	8	0.18
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	8	0.18
(3,409)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	8	0.18
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	8	0.18
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	8	0.18
(3,409)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	8	0.18
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	8	0.18
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	8	0.18
(3,409)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	8	0.18
(3,408)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	3	0.18
(3,408)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	3	0.18
(3,408)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	3	0.18
(3,408)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	3	0.18
(3,408)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,408)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	3	0.18
(3,406)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	10	0.18
(3,406)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	10	0.18
(3,406)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	10	0.18
(3,338)	1:14:A:GLN:HE22	1:21:A:ARG:HG3	1	0.18
(3,318)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.18
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	3	0.18
(3,300)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	5	0.18
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	7	0.18
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	7	0.18
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	7	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	7	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	7	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	7	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	9	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	9	0.18
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	9	0.18
(3,46)	1:6:A:ARG:HA	1:6:A:ARG:HD3	7	0.18
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	8	0.18
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	8	0.18
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	8	0.18
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	8	0.18
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	8	0.18
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	8	0.18
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	8	0.18
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	8	0.18
(2,443)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	8	0.18
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	8	0.18
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	8	0.18
(2,443)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	8	0.18
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	8	0.18
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	8	0.18
(2,443)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	8	0.18
(2,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	3	0.18
(2,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	3	0.18
(2,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	3	0.18
(2,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	3	0.18
(2,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	3	0.18
(2,440)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	10	0.18
(2,440)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	10	0.18
(2,440)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	10	0.18
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG21	2	0.18
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG22	2	0.18
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG23	2	0.18
(2,361)	1:14:A:GLN:HE22	1:21:A:ARG:HG3	1	0.18
(2,340)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.18
(2,333)	1:12:A:LEU:HB3	1:13:A:LYS:H	3	0.18
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	5	0.18
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	7	0.18
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	7	0.18
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	7	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	7	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	7	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	7	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	9	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	9	0.18
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	9	0.18
(2,49)	1:6:A:ARG:HA	1:6:A:ARG:HD3	7	0.18
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	2	0.18
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	2	0.18
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	2	0.18
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	2	0.18
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	3	0.18
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	3	0.18
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	3	0.18
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	3	0.18
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	5	0.18
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	5	0.18
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	5	0.18
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	5	0.18
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:7:A:LEU:HA	1:10:A:GLN:HB3	8	0.18
(1,447)	1:5:A:VAL:HG11	1:9:A:ILE:HD11	8	0.18
(1,447)	1:5:A:VAL:HG11	1:9:A:ILE:HD12	8	0.18
(1,447)	1:5:A:VAL:HG11	1:9:A:ILE:HD13	8	0.18
(1,447)	1:5:A:VAL:HG12	1:9:A:ILE:HD11	8	0.18
(1,447)	1:5:A:VAL:HG12	1:9:A:ILE:HD12	8	0.18
(1,447)	1:5:A:VAL:HG12	1:9:A:ILE:HD13	8	0.18
(1,447)	1:5:A:VAL:HG13	1:9:A:ILE:HD11	8	0.18
(1,447)	1:5:A:VAL:HG13	1:9:A:ILE:HD12	8	0.18
(1,447)	1:5:A:VAL:HG13	1:9:A:ILE:HD13	8	0.18
(1,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	8	0.18
(1,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	8	0.18
(1,447)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	8	0.18
(1,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	8	0.18
(1,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	8	0.18
(1,447)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	8	0.18
(1,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	8	0.18
(1,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	8	0.18
(1,447)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	8	0.18
(1,431)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	4	0.18
(1,431)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	4	0.18
(1,431)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	4	0.18
(1,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	2	0.18
(1,420)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	6	0.18
(1,420)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	6	0.18
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD21	10	0.18
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD22	10	0.18
(1,401)	1:6:A:ARG:HD3	1:7:A:LEU:HD23	10	0.18
(1,381)	1:6:A:ARG:HA	1:9:A:ILE:HB	3	0.18
(1,380)	1:8:A:TYR:HA	1:24:A:PRO:HG3	2	0.18
(1,377)	1:8:A:TYR:HA	1:11:A:TRP:HB3	10	0.18
(1,354)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	2	0.18
(1,329)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	3	0.18
(1,329)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	3	0.18
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	2	0.18
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	2	0.18
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	7	0.18
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	7	0.18
(1,275)	1:21:A:ARG:HA	1:22:A:PRO:HD3	4	0.18
(1,236)	1:23:A:PRO:HA	1:23:A:PRO:HB2	6	0.18
(1,221)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	2	0.18
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	3	0.18
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	5	0.18
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	5	0.18
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	7	0.18
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	7	0.18
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	10	0.18
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	10	0.18
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG2	1	0.18
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG3	1	0.18
(1,146)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	8	0.18
(1,133)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	6	0.18
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	6	0.18
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	6	0.18
(1,111)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	6	0.18
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG21	8	0.18
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG22	8	0.18
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG23	8	0.18
(1,94)	1:7:A:LEU:H	1:8:A:TYR:H	2	0.18
(1,94)	1:7:A:LEU:H	1:8:A:TYR:H	4	0.18
(1,30)	1:4:A:ALA:HA	1:5:A:VAL:H	7	0.18
(1,7)	1:19:A:SER:H	1:19:A:SER:HA	1	0.18
(1,7)	1:19:A:SER:H	1:19:A:SER:HA	7	0.18
(4,25)	1:7:A:LEU:HD11	1:8:A:TYR:H	10	0.17
(4,25)	1:7:A:LEU:HD12	1:8:A:TYR:H	10	0.17
(4,25)	1:7:A:LEU:HD13	1:8:A:TYR:H	10	0.17
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG11	8	0.17
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG12	8	0.17
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG13	8	0.17
(3,393)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	2	0.17
(3,117)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.17
(3,117)	1:10:A:GLN:H	1:10:A:GLN:HG2	9	0.17
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	3	0.17
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	3	0.17
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	3	0.17
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	6	0.17
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	6	0.17
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	6	0.17
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	2	0.17
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	2	0.17
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	2	0.17
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.17
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.17
(3,35)	1:5:A:VAL:H	1:5:A:VAL:HB	8	0.17
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG11	8	0.17
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG12	8	0.17
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG13	8	0.17
(2,427)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	2	0.17
(2,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	10	0.17
(2,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	10	0.17
(2,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	10	0.17
(2,129)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.17
(2,129)	1:10:A:GLN:H	1:10:A:GLN:HG2	9	0.17
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	3	0.17
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	3	0.17
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	3	0.17
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	6	0.17
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	6	0.17
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	6	0.17
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	2	0.17
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	2	0.17
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	2	0.17
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.17
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.17
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.17
(2,36)	1:5:A:VAL:H	1:5:A:VAL:HB	8	0.17
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	1	0.17
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	1	0.17
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	1	0.17
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	1	0.17
(1,384)	1:7:A:LEU:HD11	1:8:A:TYR:HA	3	0.17
(1,384)	1:7:A:LEU:HD12	1:8:A:TYR:HA	3	0.17
(1,384)	1:7:A:LEU:HD13	1:8:A:TYR:HA	3	0.17
(1,376)	1:8:A:TYR:HA	1:24:A:PRO:HD3	5	0.17
(1,347)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	8	0.17
(1,344)	1:14:A:GLN:HE21	1:14:A:GLN:HG3	4	0.17
(1,313)	1:11:A:TRP:HE3	1:12:A:LEU:H	7	0.17
(1,275)	1:21:A:ARG:HA	1:22:A:PRO:HD3	5	0.17
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	6	0.17
(1,212)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	6	0.17
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG2	4	0.17
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG3	4	0.17
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB2	9	0.17
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	7	0.17
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	7	0.17
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	7	0.17
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	7	0.17
(1,156)	1:12:A:LEU:HA	1:12:A:LEU:HB2	6	0.17
(1,144)	1:11:A:TRP:H	1:11:A:TRP:HB2	3	0.17
(1,124)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	1	0.17
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG21	1	0.17
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG22	1	0.17
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG23	1	0.17
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.17
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.17
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.17
(1,56)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	3	0.17
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB1	3	0.17
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB2	3	0.17
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB3	3	0.17
(1,25)	1:3:A:GLU:HG2	1:4:A:ALA:HA	8	0.17
(1,25)	1:3:A:GLU:HG3	1:4:A:ALA:HA	8	0.17
(1,7)	1:19:A:SER:H	1:19:A:SER:HA	2	0.17
(1,7)	1:19:A:SER:H	1:19:A:SER:HA	6	0.17
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	10	0.16
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	10	0.16
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	10	0.16
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	10	0.16
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	10	0.16
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	10	0.16
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG21	7	0.16
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG22	7	0.16
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG23	7	0.16
(4,17)	1:22:A:PRO:HA	1:22:A:PRO:HD3	1	0.16
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	7	0.16
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	7	0.16
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	7	0.16
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD21	7	0.16
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD22	7	0.16
(4,7)	1:7:A:LEU:H	1:7:A:LEU:HD23	7	0.16
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG11	4	0.16
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG12	4	0.16
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG13	4	0.16
(3,423)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.16
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB2	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB3	8	0.16
(3,413)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	5	0.16
(3,413)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	5	0.16
(3,413)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	7	0.16
(3,413)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	7	0.16
(3,406)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	3	0.16
(3,406)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	3	0.16
(3,406)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	3	0.16
(3,406)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	7	0.16
(3,406)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	7	0.16
(3,406)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	7	0.16
(3,403)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	10	0.16
(3,403)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	10	0.16
(3,403)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	10	0.16
(3,363)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	9	0.16
(3,328)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	10	0.16
(3,314)	1:7:A:LEU:HB3	1:8:A:TYR:H	7	0.16
(3,313)	1:12:A:LEU:HG	1:13:A:LYS:H	8	0.16
(3,248)	1:24:A:PRO:HA	1:24:A:PRO:HD3	5	0.16
(3,117)	1:10:A:GLN:H	1:10:A:GLN:HG2	2	0.16
(3,117)	1:10:A:GLN:H	1:10:A:GLN:HG2	4	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	1	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	1	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	1	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	2	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	2	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	2	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	4	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	4	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	4	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	5	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	5	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	5	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	9	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	9	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	9	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.16
(3,103)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.16
(3,96)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.16
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.16
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,81)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.16
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	10	0.16
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	10	0.16
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	10	0.16
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	10	0.16
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	10	0.16
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	10	0.16
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG11	4	0.16
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG12	4	0.16
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG13	4	0.16
(2,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.16
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB2	8	0.16
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB3	8	0.16
(2,450)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	5	0.16
(2,450)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	5	0.16
(2,450)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	7	0.16
(2,450)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	7	0.16
(2,440)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	3	0.16
(2,440)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	3	0.16
(2,440)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	3	0.16
(2,440)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	7	0.16
(2,440)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	7	0.16
(2,440)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	7	0.16
(2,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	10	0.16
(2,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	10	0.16
(2,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	10	0.16
(2,389)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	9	0.16
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG21	7	0.16
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG22	7	0.16
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG23	7	0.16
(2,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	10	0.16
(2,335)	1:7:A:LEU:HB3	1:8:A:TYR:H	7	0.16
(2,334)	1:12:A:LEU:HG	1:13:A:LYS:H	8	0.16
(2,265)	1:24:A:PRO:HA	1:24:A:PRO:HD3	5	0.16
(2,215)	1:22:A:PRO:HA	1:22:A:PRO:HD3	1	0.16
(2,129)	1:10:A:GLN:H	1:10:A:GLN:HG2	2	0.16
(2,129)	1:10:A:GLN:H	1:10:A:GLN:HG2	4	0.16
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD11	7	0.16
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD12	7	0.16
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD13	7	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	1	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	1	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	2	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	2	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	2	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	4	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	4	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	4	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	5	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	5	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	5	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	9	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	9	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	9	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.16
(2,113)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.16
(2,106)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.16
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD21	7	0.16
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD22	7	0.16
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HD23	7	0.16
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.16
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.16
(2,87)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.16
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	4	0.16
(1,480)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	4	0.16
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	4	0.16
(1,480)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	4	0.16
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG11	1	0.16
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG12	1	0.16
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG13	1	0.16
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG21	1	0.16
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG22	1	0.16
(1,429)	1:5:A:VAL:HB	1:5:A:VAL:HG23	1	0.16
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	4	0.16
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	4	0.16
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	4	0.16
(1,397)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	4	0.16
(1,397)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	4	0.16
(1,397)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	4	0.16
(1,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	1	0.16
(1,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	5	0.16
(1,384)	1:7:A:LEU:HD11	1:8:A:TYR:HA	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:7:A:LEU:HD12	1:8:A:TYR:HA	7	0.16
(1,384)	1:7:A:LEU:HD13	1:8:A:TYR:HA	7	0.16
(1,380)	1:8:A:TYR:HA	1:24:A:PRO:HG3	6	0.16
(1,292)	1:11:A:TRP:HA	1:11:A:TRP:HD1	5	0.16
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD2	2	0.16
(1,276)	1:21:A:ARG:HA	1:21:A:ARG:HD3	2	0.16
(1,252)	1:23:A:PRO:HA	1:24:A:PRO:HD3	9	0.16
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG2	9	0.16
(1,204)	1:17:A:PRO:HA	1:17:A:PRO:HG3	9	0.16
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB2	3	0.16
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	3	0.16
(1,156)	1:12:A:LEU:HA	1:12:A:LEU:HB2	10	0.16
(1,150)	1:15:A:GLY:HA2	1:16:A:GLY:H	8	0.16
(1,124)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	2	0.16
(1,124)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	3	0.16
(1,124)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	4	0.16
(1,124)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	5	0.16
(1,124)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	6	0.16
(1,124)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	7	0.16
(1,124)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	8	0.16
(1,124)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	9	0.16
(1,124)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	10	0.16
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG21	4	0.16
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG22	4	0.16
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG23	4	0.16
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.16
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.16
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.16
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	3	0.15
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	3	0.15
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	3	0.15
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	3	0.15
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	3	0.15
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	3	0.15
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	9	0.15
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	9	0.15
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	9	0.15
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	9	0.15
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	9	0.15
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	9	0.15
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG21	4	0.15
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG22	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG23	4	0.15
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG21	9	0.15
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG22	9	0.15
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG23	9	0.15
(4,25)	1:7:A:LEU:HD11	1:8:A:TYR:H	7	0.15
(4,25)	1:7:A:LEU:HD12	1:8:A:TYR:H	7	0.15
(4,25)	1:7:A:LEU:HD13	1:8:A:TYR:H	7	0.15
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	8	0.15
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	8	0.15
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	8	0.15
(4,3)	1:6:A:ARG:HA	1:6:A:ARG:HD2	5	0.15
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD21	7	0.15
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD22	7	0.15
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD23	7	0.15
(3,423)	1:7:A:LEU:HA	1:10:A:GLN:HB2	1	0.15
(3,423)	1:7:A:LEU:HA	1:10:A:GLN:HB2	5	0.15
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.15
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB3	2	0.15
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB2	4	0.15
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB3	4	0.15
(3,408)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	5	0.15
(3,408)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	5	0.15
(3,408)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	5	0.15
(3,408)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	5	0.15
(3,408)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	5	0.15
(3,408)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	5	0.15
(3,406)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	8	0.15
(3,406)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	8	0.15
(3,406)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	8	0.15
(3,403)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	8	0.15
(3,403)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	8	0.15
(3,403)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	8	0.15
(3,270)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	9	0.15
(3,264)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	3	0.15
(3,248)	1:24:A:PRO:HA	1:24:A:PRO:HD3	9	0.15
(3,117)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.15
(3,96)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.15
(3,96)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.15
(3,96)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.15
(3,96)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.15
(3,96)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.15
(3,96)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,96)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.15
(3,35)	1:5:A:VAL:H	1:5:A:VAL:HB	7	0.15
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	3	0.15
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	3	0.15
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	3	0.15
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	3	0.15
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	3	0.15
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	3	0.15
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	9	0.15
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	9	0.15
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	9	0.15
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	9	0.15
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	9	0.15
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	9	0.15
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD21	7	0.15
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD22	7	0.15
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD23	7	0.15
(2,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	1	0.15
(2,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	5	0.15
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.15
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB3	2	0.15
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB2	4	0.15
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB3	4	0.15
(2,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	5	0.15
(2,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	5	0.15
(2,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	5	0.15
(2,442)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	5	0.15
(2,442)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	5	0.15
(2,442)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	5	0.15
(2,440)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	8	0.15
(2,440)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	8	0.15
(2,440)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	8	0.15
(2,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	8	0.15
(2,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	8	0.15
(2,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	8	0.15
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG21	4	0.15
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG22	4	0.15
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG23	4	0.15
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG21	9	0.15
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG22	9	0.15
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG23	9	0.15
(2,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	7	0.15
(2,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	7	0.15
(2,287)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	9	0.15
(2,281)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	3	0.15
(2,265)	1:24:A:PRO:HA	1:24:A:PRO:HD3	9	0.15
(2,129)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.15
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD11	8	0.15
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD12	8	0.15
(2,119)	1:9:A:ILE:H	1:9:A:ILE:HD13	8	0.15
(2,106)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.15
(2,106)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.15
(2,106)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.15
(2,106)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.15
(2,106)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.15
(2,106)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.15
(2,106)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.15
(2,48)	1:6:A:ARG:HA	1:6:A:ARG:HD2	5	0.15
(2,36)	1:5:A:VAL:H	1:5:A:VAL:HB	7	0.15
(1,414)	1:12:A:LEU:HA	1:17:A:PRO:HD2	8	0.15
(1,409)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	7	0.15
(1,409)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	9	0.15
(1,398)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	10	0.15
(1,398)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	10	0.15
(1,398)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	10	0.15
(1,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	2	0.15
(1,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	4	0.15
(1,384)	1:7:A:LEU:HD11	1:8:A:TYR:HA	4	0.15
(1,384)	1:7:A:LEU:HD12	1:8:A:TYR:HA	4	0.15
(1,384)	1:7:A:LEU:HD13	1:8:A:TYR:HA	4	0.15
(1,384)	1:7:A:LEU:HD11	1:8:A:TYR:HA	6	0.15
(1,384)	1:7:A:LEU:HD12	1:8:A:TYR:HA	6	0.15
(1,384)	1:7:A:LEU:HD13	1:8:A:TYR:HA	6	0.15
(1,375)	1:8:A:TYR:HA	1:11:A:TRP:HB2	10	0.15
(1,344)	1:14:A:GLN:HE21	1:14:A:GLN:HG3	10	0.15
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	7	0.15
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	7	0.15
(1,292)	1:11:A:TRP:HA	1:11:A:TRP:HD1	2	0.15
(1,289)	1:15:A:GLY:H	1:16:A:GLY:H	10	0.15
(1,288)	1:13:A:LYS:H	1:14:A:GLN:H	7	0.15
(1,272)	1:20:A:GLY:H	1:20:A:GLY:HA3	5	0.15
(1,260)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	3	0.15
(1,260)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,260)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	5	0.15
(1,260)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	9	0.15
(1,188)	1:14:A:GLN:H	1:14:A:GLN:HG3	9	0.15
(1,162)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	3	0.15
(1,162)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	6	0.15
(1,162)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	8	0.15
(1,156)	1:12:A:LEU:HA	1:12:A:LEU:HB2	7	0.15
(1,146)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	7	0.15
(1,144)	1:11:A:TRP:H	1:11:A:TRP:HB2	4	0.15
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB2	8	0.15
(1,126)	1:10:A:GLN:H	1:10:A:GLN:HB3	8	0.15
(1,110)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	3	0.15
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	3	0.15
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	10	0.15
(1,52)	1:6:A:ARG:HA	1:6:A:ARG:HG2	2	0.15
(1,52)	1:6:A:ARG:HA	1:6:A:ARG:HG2	4	0.15
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB1	9	0.15
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB2	9	0.15
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB3	9	0.15
(1,7)	1:19:A:SER:H	1:19:A:SER:HA	9	0.15
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	5	0.14
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	5	0.14
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	5	0.14
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	5	0.14
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	5	0.14
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	5	0.14
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG21	1	0.14
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG22	1	0.14
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG23	1	0.14
(4,25)	1:7:A:LEU:HD11	1:8:A:TYR:H	6	0.14
(4,25)	1:7:A:LEU:HD12	1:8:A:TYR:H	6	0.14
(4,25)	1:7:A:LEU:HD13	1:8:A:TYR:H	6	0.14
(3,423)	1:7:A:LEU:HA	1:10:A:GLN:HB2	4	0.14
(3,423)	1:7:A:LEU:HA	1:10:A:GLN:HB2	6	0.14
(3,413)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	6	0.14
(3,413)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	6	0.14
(3,403)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	3	0.14
(3,403)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	3	0.14
(3,403)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	3	0.14
(3,403)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	7	0.14
(3,403)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	7	0.14
(3,403)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,402)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	2	0.14
(3,402)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	2	0.14
(3,402)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	2	0.14
(3,386)	1:12:A:LEU:HG	1:13:A:LYS:HE2	10	0.14
(3,386)	1:12:A:LEU:HG	1:13:A:LYS:HE3	10	0.14
(3,328)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	9	0.14
(3,326)	1:22:A:PRO:HG2	1:25:A:SER:H	9	0.14
(3,326)	1:22:A:PRO:HG3	1:25:A:SER:H	9	0.14
(3,313)	1:12:A:LEU:HG	1:13:A:LYS:H	3	0.14
(3,248)	1:24:A:PRO:HA	1:24:A:PRO:HD3	10	0.14
(3,174)	1:14:A:GLN:H	1:14:A:GLN:HG2	8	0.14
(3,117)	1:10:A:GLN:H	1:10:A:GLN:HG2	1	0.14
(3,117)	1:10:A:GLN:H	1:10:A:GLN:HG2	5	0.14
(3,96)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.14
(3,96)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.14
(3,21)	1:3:A:GLU:H	1:3:A:GLU:HB2	7	0.14
(3,21)	1:3:A:GLU:H	1:3:A:GLU:HB2	8	0.14
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	5	0.14
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	5	0.14
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	5	0.14
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	5	0.14
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	5	0.14
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	5	0.14
(2,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	4	0.14
(2,463)	1:7:A:LEU:HA	1:10:A:GLN:HB2	6	0.14
(2,450)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	6	0.14
(2,450)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	6	0.14
(2,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	3	0.14
(2,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	3	0.14
(2,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	3	0.14
(2,437)	1:7:A:LEU:HD11	1:24:A:PRO:HG2	7	0.14
(2,437)	1:7:A:LEU:HD12	1:24:A:PRO:HG2	7	0.14
(2,437)	1:7:A:LEU:HD13	1:24:A:PRO:HG2	7	0.14
(2,436)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	2	0.14
(2,436)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	2	0.14
(2,436)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	2	0.14
(2,418)	1:12:A:LEU:HG	1:13:A:LYS:HE2	10	0.14
(2,418)	1:12:A:LEU:HG	1:13:A:LYS:HE3	10	0.14
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG21	1	0.14
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG22	1	0.14
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG23	1	0.14
(2,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	6	0.14
(2,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	6	0.14
(2,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	9	0.14
(2,348)	1:22:A:PRO:HG2	1:25:A:SER:H	9	0.14
(2,348)	1:22:A:PRO:HG3	1:25:A:SER:H	9	0.14
(2,334)	1:12:A:LEU:HG	1:13:A:LYS:H	3	0.14
(2,265)	1:24:A:PRO:HA	1:24:A:PRO:HD3	10	0.14
(2,187)	1:14:A:GLN:H	1:14:A:GLN:HG2	8	0.14
(2,129)	1:10:A:GLN:H	1:10:A:GLN:HG2	1	0.14
(2,129)	1:10:A:GLN:H	1:10:A:GLN:HG2	5	0.14
(2,106)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.14
(2,106)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.14
(2,22)	1:3:A:GLU:H	1:3:A:GLU:HB2	7	0.14
(2,22)	1:3:A:GLU:H	1:3:A:GLU:HB2	8	0.14
(1,462)	1:11:A:TRP:HH2	1:17:A:PRO:HA	10	0.14
(1,431)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	1	0.14
(1,431)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	1	0.14
(1,431)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	1	0.14
(1,421)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	6	0.14
(1,421)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	6	0.14
(1,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	9	0.14
(1,384)	1:7:A:LEU:HD11	1:8:A:TYR:HA	9	0.14
(1,384)	1:7:A:LEU:HD12	1:8:A:TYR:HA	9	0.14
(1,384)	1:7:A:LEU:HD13	1:8:A:TYR:HA	9	0.14
(1,354)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	7	0.14
(1,344)	1:14:A:GLN:HE21	1:14:A:GLN:HG3	5	0.14
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	6	0.14
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	6	0.14
(1,312)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	6	0.14
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	6	0.14
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	6	0.14
(1,312)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	6	0.14
(1,275)	1:21:A:ARG:HA	1:22:A:PRO:HD3	9	0.14
(1,260)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	1	0.14
(1,253)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	4	0.14
(1,252)	1:23:A:PRO:HA	1:24:A:PRO:HD3	8	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	1	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	1	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	2	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	2	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	3	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	4	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	4	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	5	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	5	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	7	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	7	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	8	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	8	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	9	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	9	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	10	0.14
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	10	0.14
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB2	5	0.14
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	5	0.14
(1,162)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	9	0.14
(1,162)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.14
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD21	7	0.14
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD22	7	0.14
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD23	7	0.14
(1,156)	1:12:A:LEU:HA	1:12:A:LEU:HB2	3	0.14
(1,144)	1:11:A:TRP:H	1:11:A:TRP:HB2	9	0.14
(1,110)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	1	0.14
(1,110)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	2	0.14
(1,110)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	4	0.14
(1,110)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	5	0.14
(1,110)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	6	0.14
(1,110)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	9	0.14
(1,110)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	10	0.14
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG21	2	0.14
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG22	2	0.14
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG23	2	0.14
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG21	5	0.14
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG22	5	0.14
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG23	5	0.14
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG21	9	0.14
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG22	9	0.14
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG23	9	0.14
(1,72)	1:6:A:ARG:HD3	1:7:A:LEU:H	4	0.14
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB1	2	0.14
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB2	2	0.14
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB3	2	0.14
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB1	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB2	7	0.14
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB3	7	0.14
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB1	8	0.14
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB2	8	0.14
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB3	8	0.14
(1,7)	1:19:A:SER:H	1:19:A:SER:HA	3	0.14
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG21	8	0.13
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG22	8	0.13
(4,26)	1:6:A:ARG:HA	1:9:A:ILE:HG23	8	0.13
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD21	5	0.13
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD22	5	0.13
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD23	5	0.13
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG11	2	0.13
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG12	2	0.13
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG13	2	0.13
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG11	5	0.13
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG12	5	0.13
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG13	5	0.13
(3,424)	1:3:A:GLU:HA	1:6:A:ARG:HB2	6	0.13
(3,424)	1:3:A:GLU:HA	1:6:A:ARG:HB2	7	0.13
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB2	1	0.13
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB3	1	0.13
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB2	6	0.13
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB3	6	0.13
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB2	7	0.13
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB3	7	0.13
(3,406)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	5	0.13
(3,406)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	5	0.13
(3,406)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	5	0.13
(3,406)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	6	0.13
(3,406)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	6	0.13
(3,406)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	6	0.13
(3,402)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	1	0.13
(3,402)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	1	0.13
(3,402)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	1	0.13
(3,361)	1:5:A:VAL:HA	1:8:A:TYR:HB2	3	0.13
(3,361)	1:5:A:VAL:HA	1:8:A:TYR:HB2	9	0.13
(3,345)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	7	0.13
(3,345)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	7	0.13
(3,345)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	7	0.13
(3,345)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	7	0.13
(3,345)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,345)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	7	0.13
(3,345)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	7	0.13
(3,345)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	7	0.13
(3,345)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	7	0.13
(3,345)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	7	0.13
(3,345)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	7	0.13
(3,345)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	7	0.13
(3,331)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	2	0.13
(3,328)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	5	0.13
(3,264)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	7	0.13
(3,193)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	5	0.13
(3,193)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	10	0.13
(3,83)	1:7:A:LEU:H	1:7:A:LEU:HG	7	0.13
(3,46)	1:6:A:ARG:HA	1:6:A:ARG:HD3	8	0.13
(3,32)	1:4:A:ALA:HB1	1:5:A:VAL:H	6	0.13
(3,32)	1:4:A:ALA:HB2	1:5:A:VAL:H	6	0.13
(3,32)	1:4:A:ALA:HB3	1:5:A:VAL:H	6	0.13
(3,21)	1:3:A:GLU:H	1:3:A:GLU:HB2	10	0.13
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD21	5	0.13
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD22	5	0.13
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD23	5	0.13
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG11	2	0.13
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG12	2	0.13
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG13	2	0.13
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG11	5	0.13
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG12	5	0.13
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG13	5	0.13
(2,464)	1:3:A:GLU:HA	1:6:A:ARG:HB2	6	0.13
(2,464)	1:3:A:GLU:HA	1:6:A:ARG:HB2	7	0.13
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB2	1	0.13
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB3	1	0.13
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB2	6	0.13
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB3	6	0.13
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB2	7	0.13
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB3	7	0.13
(2,440)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	5	0.13
(2,440)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	5	0.13
(2,440)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	5	0.13
(2,440)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	6	0.13
(2,440)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	6	0.13
(2,440)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	6	0.13
(2,436)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,436)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	1	0.13
(2,436)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	1	0.13
(2,387)	1:5:A:VAL:HA	1:8:A:TYR:HB2	3	0.13
(2,387)	1:5:A:VAL:HA	1:8:A:TYR:HB2	9	0.13
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG21	8	0.13
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG22	8	0.13
(2,383)	1:6:A:ARG:HA	1:9:A:ILE:HG23	8	0.13
(2,369)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	7	0.13
(2,369)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	7	0.13
(2,369)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	7	0.13
(2,369)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	7	0.13
(2,369)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	7	0.13
(2,369)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	7	0.13
(2,369)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	7	0.13
(2,369)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	7	0.13
(2,369)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	7	0.13
(2,369)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	7	0.13
(2,369)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	7	0.13
(2,369)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	7	0.13
(2,353)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	2	0.13
(2,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	5	0.13
(2,281)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	7	0.13
(2,208)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	5	0.13
(2,208)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	10	0.13
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HG	7	0.13
(2,49)	1:6:A:ARG:HA	1:6:A:ARG:HD3	8	0.13
(2,33)	1:4:A:ALA:HB1	1:5:A:VAL:H	6	0.13
(2,33)	1:4:A:ALA:HB2	1:5:A:VAL:H	6	0.13
(2,33)	1:4:A:ALA:HB3	1:5:A:VAL:H	6	0.13
(2,22)	1:3:A:GLU:H	1:3:A:GLU:HB2	10	0.13
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB1	5	0.13
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB2	5	0.13
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB3	5	0.13
(1,459)	1:11:A:TRP:HE3	1:12:A:LEU:HB2	7	0.13
(1,407)	1:12:A:LEU:HD21	1:17:A:PRO:HD2	5	0.13
(1,407)	1:12:A:LEU:HD22	1:17:A:PRO:HD2	5	0.13
(1,407)	1:12:A:LEU:HD23	1:17:A:PRO:HD2	5	0.13
(1,391)	1:9:A:ILE:HA	1:12:A:LEU:HB3	10	0.13
(1,384)	1:7:A:LEU:HD11	1:8:A:TYR:HA	1	0.13
(1,384)	1:7:A:LEU:HD12	1:8:A:TYR:HA	1	0.13
(1,384)	1:7:A:LEU:HD13	1:8:A:TYR:HA	1	0.13
(1,380)	1:8:A:TYR:HA	1:24:A:PRO:HG3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	5	0.13
(1,296)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	5	0.13
(1,292)	1:11:A:TRP:HA	1:11:A:TRP:HD1	9	0.13
(1,260)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	2	0.13
(1,260)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	7	0.13
(1,253)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	1	0.13
(1,253)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	2	0.13
(1,253)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	6	0.13
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	6	0.13
(1,227)	1:22:A:PRO:HB2	1:22:A:PRO:HG3	6	0.13
(1,225)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	1	0.13
(1,189)	1:14:A:GLN:HA	1:14:A:GLN:HG3	8	0.13
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB2	4	0.13
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	4	0.13
(1,162)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	1	0.13
(1,162)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	2	0.13
(1,162)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	4	0.13
(1,162)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	5	0.13
(1,162)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	7	0.13
(1,156)	1:12:A:LEU:HA	1:12:A:LEU:HB2	8	0.13
(1,150)	1:15:A:GLY:HA2	1:16:A:GLY:H	6	0.13
(1,144)	1:11:A:TRP:H	1:11:A:TRP:HB2	1	0.13
(1,144)	1:11:A:TRP:H	1:11:A:TRP:HB2	5	0.13
(1,144)	1:11:A:TRP:H	1:11:A:TRP:HB2	8	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG21	2	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG22	2	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG23	2	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG21	5	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG22	5	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG23	5	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG21	6	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG22	6	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG23	6	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG21	7	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG22	7	0.13
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG23	7	0.13
(1,94)	1:7:A:LEU:H	1:8:A:TYR:H	9	0.13
(1,52)	1:6:A:ARG:HA	1:6:A:ARG:HG2	8	0.13
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB1	4	0.13
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB2	4	0.13
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB3	4	0.13
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB1	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB2	5	0.13
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB3	5	0.13
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB1	6	0.13
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB2	6	0.13
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB3	6	0.13
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB1	10	0.13
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB2	10	0.13
(1,29)	1:4:A:ALA:H	1:4:A:ALA:HB3	10	0.13
(1,26)	1:3:A:GLU:HG2	1:4:A:ALA:H	8	0.13
(1,26)	1:3:A:GLU:HG3	1:4:A:ALA:H	8	0.13
(1,23)	1:3:A:GLU:H	1:3:A:GLU:HB3	1	0.13
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	6	0.12
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	6	0.12
(4,42)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	6	0.12
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	6	0.12
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	6	0.12
(4,42)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	6	0.12
(4,31)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	6	0.12
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD21	6	0.12
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD22	6	0.12
(3,434)	1:4:A:ALA:H	1:7:A:LEU:HD23	6	0.12
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG11	6	0.12
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG12	6	0.12
(3,427)	1:4:A:ALA:HA	1:5:A:VAL:HG13	6	0.12
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB2	9	0.12
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB3	9	0.12
(3,402)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	4	0.12
(3,402)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	4	0.12
(3,402)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	4	0.12
(3,398)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	6	0.12
(3,398)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	6	0.12
(3,398)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	6	0.12
(3,398)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	6	0.12
(3,398)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	6	0.12
(3,398)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	6	0.12
(3,345)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	4	0.12
(3,345)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	4	0.12
(3,345)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	4	0.12
(3,345)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	4	0.12
(3,345)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	4	0.12
(3,345)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	4	0.12
(3,345)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,345)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	4	0.12
(3,345)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	4	0.12
(3,345)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	4	0.12
(3,345)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	4	0.12
(3,345)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	4	0.12
(3,329)	1:13:A:LYS:HB2	1:14:A:GLN:H	4	0.12
(3,327)	1:24:A:PRO:HB3	1:25:A:SER:H	3	0.12
(3,327)	1:24:A:PRO:HB3	1:25:A:SER:H	9	0.12
(3,326)	1:22:A:PRO:HG2	1:25:A:SER:H	2	0.12
(3,326)	1:22:A:PRO:HG3	1:25:A:SER:H	2	0.12
(3,326)	1:22:A:PRO:HG2	1:25:A:SER:H	7	0.12
(3,326)	1:22:A:PRO:HG3	1:25:A:SER:H	7	0.12
(3,326)	1:22:A:PRO:HG2	1:25:A:SER:H	10	0.12
(3,326)	1:22:A:PRO:HG3	1:25:A:SER:H	10	0.12
(3,248)	1:24:A:PRO:HA	1:24:A:PRO:HD3	4	0.12
(3,110)	1:8:A:TYR:HA	1:10:A:GLN:H	7	0.12
(3,46)	1:6:A:ARG:HA	1:6:A:ARG:HD3	2	0.12
(3,32)	1:4:A:ALA:HB1	1:5:A:VAL:H	5	0.12
(3,32)	1:4:A:ALA:HB2	1:5:A:VAL:H	5	0.12
(3,32)	1:4:A:ALA:HB3	1:5:A:VAL:H	5	0.12
(3,32)	1:4:A:ALA:HB1	1:5:A:VAL:H	9	0.12
(3,32)	1:4:A:ALA:HB2	1:5:A:VAL:H	9	0.12
(3,32)	1:4:A:ALA:HB3	1:5:A:VAL:H	9	0.12
(3,21)	1:3:A:GLU:H	1:3:A:GLU:HB2	2	0.12
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD21	6	0.12
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD22	6	0.12
(2,484)	1:3:A:GLU:HG2	1:7:A:LEU:HD23	6	0.12
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	6	0.12
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	6	0.12
(2,484)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	6	0.12
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD21	6	0.12
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD22	6	0.12
(2,475)	1:4:A:ALA:H	1:7:A:LEU:HD23	6	0.12
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG11	6	0.12
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG12	6	0.12
(2,467)	1:4:A:ALA:HA	1:5:A:VAL:HG13	6	0.12
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB2	9	0.12
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB3	9	0.12
(2,436)	1:7:A:LEU:HD21	1:24:A:PRO:HG2	4	0.12
(2,436)	1:7:A:LEU:HD22	1:24:A:PRO:HG2	4	0.12
(2,436)	1:7:A:LEU:HD23	1:24:A:PRO:HG2	4	0.12
(2,432)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,432)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	6	0.12
(2,432)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	6	0.12
(2,432)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	6	0.12
(2,432)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	6	0.12
(2,432)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	6	0.12
(2,415)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	6	0.12
(2,369)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	4	0.12
(2,369)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	4	0.12
(2,369)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	4	0.12
(2,369)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	4	0.12
(2,369)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	4	0.12
(2,369)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	4	0.12
(2,369)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	4	0.12
(2,369)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	4	0.12
(2,369)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	4	0.12
(2,369)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	4	0.12
(2,369)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	4	0.12
(2,369)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	4	0.12
(2,351)	1:13:A:LYS:HB2	1:14:A:GLN:H	4	0.12
(2,349)	1:24:A:PRO:HB3	1:25:A:SER:H	3	0.12
(2,349)	1:24:A:PRO:HB3	1:25:A:SER:H	9	0.12
(2,348)	1:22:A:PRO:HG2	1:25:A:SER:H	2	0.12
(2,348)	1:22:A:PRO:HG3	1:25:A:SER:H	2	0.12
(2,348)	1:22:A:PRO:HG2	1:25:A:SER:H	7	0.12
(2,348)	1:22:A:PRO:HG3	1:25:A:SER:H	7	0.12
(2,348)	1:22:A:PRO:HG2	1:25:A:SER:H	10	0.12
(2,348)	1:22:A:PRO:HG3	1:25:A:SER:H	10	0.12
(2,265)	1:24:A:PRO:HA	1:24:A:PRO:HD3	4	0.12
(2,122)	1:8:A:TYR:HA	1:10:A:GLN:H	7	0.12
(2,49)	1:6:A:ARG:HA	1:6:A:ARG:HD3	2	0.12
(2,33)	1:4:A:ALA:HB1	1:5:A:VAL:H	5	0.12
(2,33)	1:4:A:ALA:HB2	1:5:A:VAL:H	5	0.12
(2,33)	1:4:A:ALA:HB3	1:5:A:VAL:H	5	0.12
(2,33)	1:4:A:ALA:HB1	1:5:A:VAL:H	9	0.12
(2,33)	1:4:A:ALA:HB2	1:5:A:VAL:H	9	0.12
(2,33)	1:4:A:ALA:HB3	1:5:A:VAL:H	9	0.12
(2,22)	1:3:A:GLU:H	1:3:A:GLU:HB2	2	0.12
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB1	4	0.12
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB2	4	0.12
(1,482)	1:1:A:GLU:HB2	1:4:A:ALA:HB3	4	0.12
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB1	4	0.12
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB2	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:1:A:GLU:HB3	1:4:A:ALA:HB3	4	0.12
(1,428)	1:16:A:GLY:HA3	1:21:A:ARG:HB3	5	0.12
(1,421)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	2	0.12
(1,421)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	2	0.12
(1,402)	1:7:A:LEU:HD21	1:8:A:TYR:HB3	4	0.12
(1,402)	1:7:A:LEU:HD22	1:8:A:TYR:HB3	4	0.12
(1,402)	1:7:A:LEU:HD23	1:8:A:TYR:HB3	4	0.12
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD21	9	0.12
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD22	9	0.12
(1,395)	1:9:A:ILE:HA	1:12:A:LEU:HD23	9	0.12
(1,381)	1:6:A:ARG:HA	1:9:A:ILE:HB	6	0.12
(1,377)	1:8:A:TYR:HA	1:11:A:TRP:HB3	5	0.12
(1,361)	1:14:A:GLN:HE22	1:21:A:ARG:HG3	3	0.12
(1,361)	1:14:A:GLN:HE22	1:21:A:ARG:HG3	4	0.12
(1,361)	1:14:A:GLN:HE22	1:21:A:ARG:HG3	8	0.12
(1,353)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	7	0.12
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	6	0.12
(1,302)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	6	0.12
(1,253)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	5	0.12
(1,253)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	7	0.12
(1,253)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	8	0.12
(1,253)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	9	0.12
(1,226)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	1	0.12
(1,226)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	2	0.12
(1,226)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	3	0.12
(1,226)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	4	0.12
(1,226)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	5	0.12
(1,226)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	6	0.12
(1,226)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	7	0.12
(1,226)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	8	0.12
(1,226)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	9	0.12
(1,226)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	10	0.12
(1,211)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	10	0.12
(1,198)	1:19:A:SER:H	1:19:A:SER:HB3	2	0.12
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB2	2	0.12
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	2	0.12
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB2	6	0.12
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	6	0.12
(1,146)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	10	0.12
(1,144)	1:11:A:TRP:H	1:11:A:TRP:HB2	2	0.12
(1,110)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	8	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG21	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG22	1	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG23	1	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG21	3	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG22	3	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG23	3	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG21	4	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG22	4	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG23	4	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG21	8	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG22	8	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG23	8	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG21	9	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG22	9	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG23	9	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG21	10	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG22	10	0.12
(1,108)	1:9:A:ILE:HB	1:9:A:ILE:HG23	10	0.12
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG21	10	0.12
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG22	10	0.12
(1,104)	1:9:A:ILE:HA	1:9:A:ILE:HG23	10	0.12
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	9	0.12
(1,57)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	2	0.12
(1,57)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	3	0.12
(1,57)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	8	0.12
(1,57)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	10	0.12
(1,37)	1:5:A:VAL:H	1:5:A:VAL:HG11	10	0.12
(1,37)	1:5:A:VAL:H	1:5:A:VAL:HG12	10	0.12
(1,37)	1:5:A:VAL:H	1:5:A:VAL:HG13	10	0.12
(1,37)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.12
(1,37)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.12
(1,37)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.12
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB1	6	0.12
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB2	6	0.12
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB3	6	0.12
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB1	8	0.12
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB2	8	0.12
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB3	8	0.12
(4,25)	1:7:A:LEU:HD11	1:8:A:TYR:H	3	0.11
(4,25)	1:7:A:LEU:HD12	1:8:A:TYR:H	3	0.11
(4,25)	1:7:A:LEU:HD13	1:8:A:TYR:H	3	0.11
(4,25)	1:7:A:LEU:HD11	1:8:A:TYR:H	5	0.11
(4,25)	1:7:A:LEU:HD12	1:8:A:TYR:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,25)	1:7:A:LEU:HD13	1:8:A:TYR:H	5	0.11
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB2	3	0.11
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB3	3	0.11
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB2	5	0.11
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB3	5	0.11
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.11
(3,420)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.11
(3,413)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	10	0.11
(3,413)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	10	0.11
(3,386)	1:12:A:LEU:HG	1:13:A:LYS:HE2	7	0.11
(3,386)	1:12:A:LEU:HG	1:13:A:LYS:HE3	7	0.11
(3,326)	1:22:A:PRO:HG2	1:25:A:SER:H	3	0.11
(3,326)	1:22:A:PRO:HG3	1:25:A:SER:H	3	0.11
(3,308)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	7	0.11
(3,308)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	7	0.11
(3,264)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	4	0.11
(3,248)	1:24:A:PRO:HA	1:24:A:PRO:HD3	3	0.11
(3,248)	1:24:A:PRO:HA	1:24:A:PRO:HD3	7	0.11
(3,193)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	8	0.11
(3,83)	1:7:A:LEU:H	1:7:A:LEU:HG	5	0.11
(3,41)	1:6:A:ARG:HA	1:7:A:LEU:H	3	0.11
(3,41)	1:6:A:ARG:HA	1:7:A:LEU:H	10	0.11
(3,38)	1:3:A:GLU:H	1:5:A:VAL:HB	7	0.11
(3,38)	1:3:A:GLU:H	1:5:A:VAL:HB	8	0.11
(3,38)	1:3:A:GLU:H	1:5:A:VAL:HB	9	0.11
(3,38)	1:3:A:GLU:H	1:5:A:VAL:HB	10	0.11
(3,32)	1:4:A:ALA:HB1	1:5:A:VAL:H	4	0.11
(3,32)	1:4:A:ALA:HB2	1:5:A:VAL:H	4	0.11
(3,32)	1:4:A:ALA:HB3	1:5:A:VAL:H	4	0.11
(3,32)	1:4:A:ALA:HB1	1:5:A:VAL:H	7	0.11
(3,32)	1:4:A:ALA:HB2	1:5:A:VAL:H	7	0.11
(3,32)	1:4:A:ALA:HB3	1:5:A:VAL:H	7	0.11
(3,21)	1:3:A:GLU:H	1:3:A:GLU:HB2	3	0.11
(3,21)	1:3:A:GLU:H	1:3:A:GLU:HB2	4	0.11
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB2	3	0.11
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB3	3	0.11
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB2	5	0.11
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB3	5	0.11
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.11
(2,458)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.11
(2,450)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	10	0.11
(2,450)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,418)	1:12:A:LEU:HG	1:13:A:LYS:HE2	7	0.11
(2,418)	1:12:A:LEU:HG	1:13:A:LYS:HE3	7	0.11
(2,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	3	0.11
(2,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	3	0.11
(2,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	3	0.11
(2,372)	1:7:A:LEU:HD11	1:8:A:TYR:H	5	0.11
(2,372)	1:7:A:LEU:HD12	1:8:A:TYR:H	5	0.11
(2,372)	1:7:A:LEU:HD13	1:8:A:TYR:H	5	0.11
(2,348)	1:22:A:PRO:HG2	1:25:A:SER:H	3	0.11
(2,348)	1:22:A:PRO:HG3	1:25:A:SER:H	3	0.11
(2,329)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	7	0.11
(2,329)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	7	0.11
(2,281)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	4	0.11
(2,265)	1:24:A:PRO:HA	1:24:A:PRO:HD3	3	0.11
(2,265)	1:24:A:PRO:HA	1:24:A:PRO:HD3	7	0.11
(2,208)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	8	0.11
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HG	5	0.11
(2,43)	1:6:A:ARG:HA	1:7:A:LEU:H	3	0.11
(2,43)	1:6:A:ARG:HA	1:7:A:LEU:H	10	0.11
(2,40)	1:3:A:GLU:H	1:5:A:VAL:HB	7	0.11
(2,40)	1:3:A:GLU:H	1:5:A:VAL:HB	8	0.11
(2,40)	1:3:A:GLU:H	1:5:A:VAL:HB	9	0.11
(2,40)	1:3:A:GLU:H	1:5:A:VAL:HB	10	0.11
(2,33)	1:4:A:ALA:HB1	1:5:A:VAL:H	4	0.11
(2,33)	1:4:A:ALA:HB2	1:5:A:VAL:H	4	0.11
(2,33)	1:4:A:ALA:HB3	1:5:A:VAL:H	4	0.11
(2,33)	1:4:A:ALA:HB1	1:5:A:VAL:H	7	0.11
(2,33)	1:4:A:ALA:HB2	1:5:A:VAL:H	7	0.11
(2,33)	1:4:A:ALA:HB3	1:5:A:VAL:H	7	0.11
(2,22)	1:3:A:GLU:H	1:3:A:GLU:HB2	3	0.11
(2,22)	1:3:A:GLU:H	1:3:A:GLU:HB2	4	0.11
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB1	3	0.11
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB2	3	0.11
(1,481)	1:1:A:GLU:HG2	1:4:A:ALA:HB3	3	0.11
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB1	3	0.11
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB2	3	0.11
(1,481)	1:1:A:GLU:HG3	1:4:A:ALA:HB3	3	0.11
(1,421)	1:14:A:GLN:HB2	1:14:A:GLN:HG2	10	0.11
(1,421)	1:14:A:GLN:HB3	1:14:A:GLN:HG2	10	0.11
(1,414)	1:12:A:LEU:HA	1:17:A:PRO:HD2	3	0.11
(1,407)	1:12:A:LEU:HD21	1:17:A:PRO:HD2	2	0.11
(1,407)	1:12:A:LEU:HD22	1:17:A:PRO:HD2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:12:A:LEU:HD23	1:17:A:PRO:HD2	2	0.11
(1,407)	1:12:A:LEU:HD21	1:17:A:PRO:HD2	4	0.11
(1,407)	1:12:A:LEU:HD22	1:17:A:PRO:HD2	4	0.11
(1,407)	1:12:A:LEU:HD23	1:17:A:PRO:HD2	4	0.11
(1,344)	1:14:A:GLN:HE21	1:14:A:GLN:HG3	9	0.11
(1,323)	1:14:A:GLN:HA	1:15:A:GLY:H	4	0.11
(1,275)	1:21:A:ARG:HA	1:22:A:PRO:HD3	1	0.11
(1,260)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	8	0.11
(1,253)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	3	0.11
(1,253)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	10	0.11
(1,249)	1:25:A:SER:H	1:25:A:SER:HB2	4	0.11
(1,249)	1:25:A:SER:H	1:25:A:SER:HB3	4	0.11
(1,211)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	8	0.11
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB2	8	0.11
(1,181)	1:13:A:LYS:H	1:13:A:LYS:HB3	8	0.11
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD21	8	0.11
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD22	8	0.11
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD23	8	0.11
(1,146)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	6	0.11
(1,110)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	7	0.11
(1,98)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	8	0.11
(1,94)	1:7:A:LEU:H	1:8:A:TYR:H	1	0.11
(1,94)	1:7:A:LEU:H	1:8:A:TYR:H	8	0.11
(1,80)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	1	0.11
(1,80)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	4	0.11
(1,80)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	5	0.11
(1,80)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	6	0.11
(1,80)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	7	0.11
(1,80)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	9	0.11
(1,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.11
(1,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.11
(1,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.11
(1,57)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	4	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB1	1	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB2	1	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB3	1	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB1	2	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB2	2	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB3	2	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB1	3	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB2	3	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB1	4	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB2	4	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB3	4	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB1	5	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB2	5	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB3	5	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB1	7	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB2	7	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB3	7	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB1	9	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB2	9	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB3	9	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB1	10	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB2	10	0.11
(1,24)	1:4:A:ALA:HA	1:4:A:ALA:HB3	10	0.11
(3,418)	1:12:A:LEU:HD11	1:13:A:LYS:H	6	0.1
(3,418)	1:12:A:LEU:HD12	1:13:A:LYS:H	6	0.1
(3,418)	1:12:A:LEU:HD13	1:13:A:LYS:H	6	0.1
(3,393)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	1	0.1
(3,345)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	5	0.1
(3,345)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	5	0.1
(3,345)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	5	0.1
(3,345)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	5	0.1
(3,345)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	5	0.1
(3,345)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	5	0.1
(3,345)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	5	0.1
(3,345)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	5	0.1
(3,345)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	5	0.1
(3,345)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	5	0.1
(3,345)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	5	0.1
(3,345)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	5	0.1
(3,329)	1:13:A:LYS:HB2	1:14:A:GLN:H	5	0.1
(3,328)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	4	0.1
(3,327)	1:24:A:PRO:HB3	1:25:A:SER:H	7	0.1
(3,193)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	3	0.1
(3,193)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	7	0.1
(3,193)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	9	0.1
(3,184)	1:19:A:SER:H	1:19:A:SER:HB3	10	0.1
(3,110)	1:8:A:TYR:HA	1:10:A:GLN:H	8	0.1
(3,32)	1:4:A:ALA:HB1	1:5:A:VAL:H	2	0.1
(3,32)	1:4:A:ALA:HB2	1:5:A:VAL:H	2	0.1
(3,32)	1:4:A:ALA:HB3	1:5:A:VAL:H	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:3:A:GLU:H	1:3:A:GLU:HB2	5	0.1
(3,21)	1:3:A:GLU:H	1:3:A:GLU:HB2	9	0.1
(2,456)	1:12:A:LEU:HD11	1:13:A:LYS:H	6	0.1
(2,456)	1:12:A:LEU:HD12	1:13:A:LYS:H	6	0.1
(2,456)	1:12:A:LEU:HD13	1:13:A:LYS:H	6	0.1
(2,427)	1:16:A:GLY:HA3	1:21:A:ARG:HB2	1	0.1
(2,369)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	5	0.1
(2,369)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	5	0.1
(2,369)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	5	0.1
(2,369)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	5	0.1
(2,369)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	5	0.1
(2,369)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	5	0.1
(2,369)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	5	0.1
(2,369)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	5	0.1
(2,369)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	5	0.1
(2,369)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	5	0.1
(2,369)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	5	0.1
(2,369)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	5	0.1
(2,351)	1:13:A:LYS:HB2	1:14:A:GLN:H	5	0.1
(2,350)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	4	0.1
(2,349)	1:24:A:PRO:HB3	1:25:A:SER:H	7	0.1
(2,208)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	3	0.1
(2,208)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	7	0.1
(2,208)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	9	0.1
(2,198)	1:19:A:SER:H	1:19:A:SER:HB3	10	0.1
(2,122)	1:8:A:TYR:HA	1:10:A:GLN:H	8	0.1
(2,33)	1:4:A:ALA:HB1	1:5:A:VAL:H	2	0.1
(2,33)	1:4:A:ALA:HB2	1:5:A:VAL:H	2	0.1
(2,33)	1:4:A:ALA:HB3	1:5:A:VAL:H	2	0.1
(2,22)	1:3:A:GLU:H	1:3:A:GLU:HB2	5	0.1
(2,22)	1:3:A:GLU:H	1:3:A:GLU:HB2	9	0.1
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB1	10	0.1
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB2	10	0.1
(1,474)	1:3:A:GLU:H	1:4:A:ALA:HB3	10	0.1
(1,399)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	3	0.1
(1,399)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	3	0.1
(1,399)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	3	0.1
(1,399)	1:5:A:VAL:HG21	1:8:A:TYR:HB3	3	0.1
(1,399)	1:5:A:VAL:HG22	1:8:A:TYR:HB3	3	0.1
(1,399)	1:5:A:VAL:HG23	1:8:A:TYR:HB3	3	0.1
(1,380)	1:8:A:TYR:HA	1:24:A:PRO:HG3	1	0.1
(1,376)	1:8:A:TYR:HA	1:24:A:PRO:HD3	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:11:A:TRP:HA	1:11:A:TRP:HD1	4	0.1
(1,221)	1:22:A:PRO:HB2	1:22:A:PRO:HD3	1	0.1
(1,211)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	5	0.1
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD21	3	0.1
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD22	3	0.1
(1,160)	1:12:A:LEU:HA	1:12:A:LEU:HD23	3	0.1
(1,147)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.1
(1,134)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	6	0.1
(1,134)	1:10:A:GLN:HB3	1:10:A:GLN:HG2	6	0.1
(1,98)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	7	0.1
(1,80)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	2	0.1
(1,80)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	3	0.1
(1,80)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	8	0.1
(1,80)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.1
(1,75)	1:7:A:LEU:HA	1:7:A:LEU:HD11	5	0.1
(1,75)	1:7:A:LEU:HA	1:7:A:LEU:HD12	5	0.1
(1,75)	1:7:A:LEU:HA	1:7:A:LEU:HD13	5	0.1
(1,73)	1:6:A:ARG:HD2	1:7:A:LEU:H	9	0.1
(1,35)	1:5:A:VAL:HA	1:5:A:VAL:HG11	1	0.1
(1,35)	1:5:A:VAL:HA	1:5:A:VAL:HG12	1	0.1
(1,35)	1:5:A:VAL:HA	1:5:A:VAL:HG13	1	0.1
(1,35)	1:5:A:VAL:HA	1:5:A:VAL:HG21	1	0.1
(1,35)	1:5:A:VAL:HA	1:5:A:VAL:HG22	1	0.1
(1,35)	1:5:A:VAL:HA	1:5:A:VAL:HG23	1	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found