



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 10:51 AM UTC

PDB ID : 9GDU / pdb_00009gdu
BMRB ID : 34945
Title : Trp-cage fortified Tc5b-Exenatide chimera with disulfide bond cyclization (Ex-4-Tc5bCC) at 310K
Authors : Horvath, D.
Deposited on : 2024-08-06

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

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

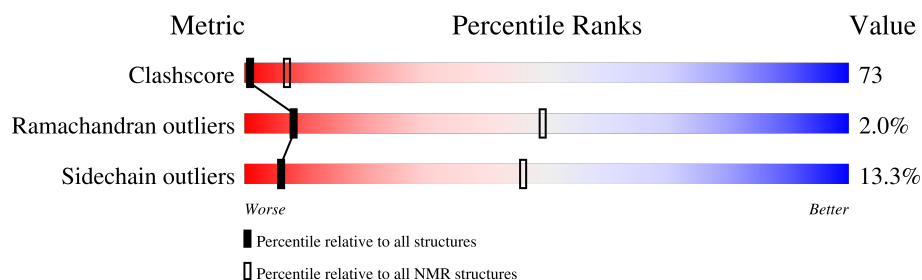
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 52%.

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	36% 40% 8% 16%

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:5-A:25 (21)	0.24	3

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

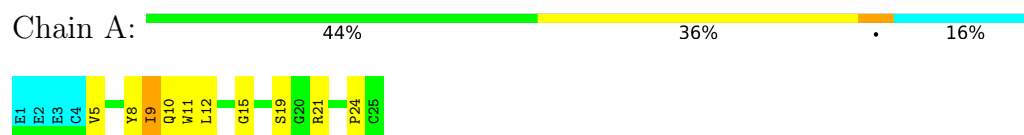
There is only 1 type of molecule in this entry. The entry contains 384 atoms, of which 187 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bCC).

Mol	Chain	Residues	Atoms						Trace
1	A	25	Total	C	H	N	O	S	0
			384	123	187	34	38	2	

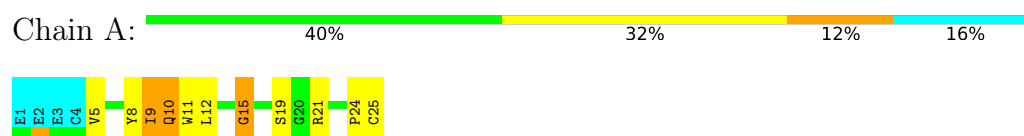
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bCC)



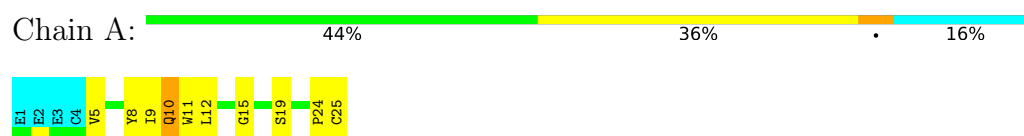
4.2.4 Score per residue for model 4

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bCC)



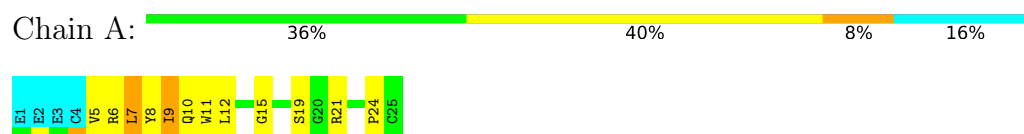
4.2.5 Score per residue for model 5

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bCC)



4.2.6 Score per residue for model 6

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bCC)



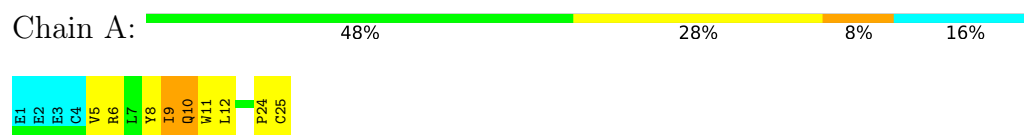
4.2.7 Score per residue for model 7

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bCC)



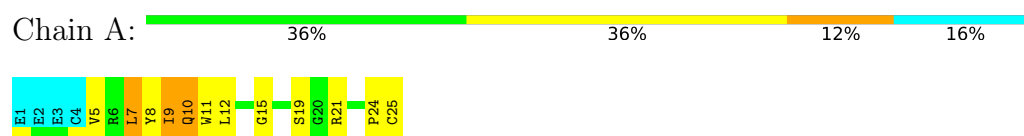
4.2.8 Score per residue for model 8

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bCC)



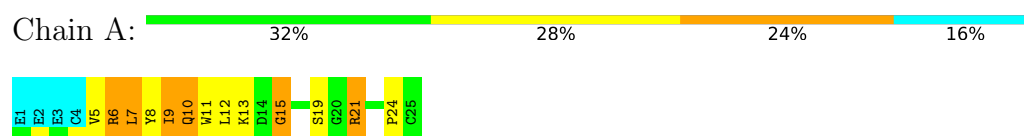
4.2.9 Score per residue for model 9

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bCC)



4.2.10 Score per residue for model 10

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bCC)



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)	52%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	164	163	163	24±3
All	All	1640	1630	1630	238

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 73.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:TYR:O	1:A:11:TRP:HB3	0.77	1.79	1	10
1:A:5:VAL:O	1:A:9:ILE:HG13	0.75	1.82	9	10
1:A:8:TYR:CE1	1:A:12:LEU:HD11	0.73	2.18	8	10
1:A:5:VAL:HG12	1:A:9:ILE:CG1	0.72	2.14	4	7
1:A:8:TYR:CZ	1:A:12:LEU:HD11	0.72	2.20	10	8
1:A:11:TRP:CE3	1:A:12:LEU:HD12	0.66	2.26	9	8
1:A:9:ILE:HA	1:A:12:LEU:HD13	0.65	1.67	9	7
1:A:5:VAL:HA	1:A:8:TYR:HB3	0.63	1.69	5	10
1:A:8:TYR:HA	1:A:24:PRO:CG	0.62	2.24	6	10
1:A:11:TRP:HE3	1:A:12:LEU:HD12	0.61	1.55	9	7
1:A:9:ILE:O	1:A:13:LYS:HD2	0.61	1.95	10	1
1:A:10:GLN:NE2	1:A:10:GLN:HA	0.59	2.12	2	10
1:A:9:ILE:HA	1:A:12:LEU:HD12	0.57	1.75	2	2
1:A:5:VAL:HG12	1:A:9:ILE:HD11	0.56	1.74	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:GLY:CA	1:A:19:SER:HB3	0.56	2.30	6	9
1:A:5:VAL:CG1	1:A:9:ILE:HD11	0.55	2.32	2	10
1:A:8:TYR:O	1:A:12:LEU:HD13	0.54	2.02	5	6
1:A:8:TYR:CE1	1:A:12:LEU:HD21	0.54	2.38	7	4
1:A:5:VAL:HG12	1:A:9:ILE:CD1	0.53	2.33	9	7
1:A:9:ILE:HG23	1:A:12:LEU:HD12	0.53	1.81	2	2
1:A:5:VAL:O	1:A:8:TYR:HB3	0.53	2.04	6	9
1:A:6:ARG:HG3	1:A:7:LEU:H	0.52	1.64	7	1
1:A:9:ILE:O	1:A:12:LEU:HB2	0.51	2.04	10	4
1:A:8:TYR:CZ	1:A:12:LEU:HD21	0.51	2.41	7	2
1:A:6:ARG:HG3	1:A:7:LEU:N	0.51	2.21	7	1
1:A:9:ILE:HA	1:A:12:LEU:CD1	0.50	2.36	2	2
1:A:9:ILE:HA	1:A:12:LEU:CG	0.48	2.38	7	2
1:A:8:TYR:HA	1:A:24:PRO:HG2	0.47	1.86	8	10
1:A:15:GLY:C	1:A:19:SER:HB3	0.47	2.34	6	6
1:A:11:TRP:CE3	1:A:12:LEU:CD1	0.47	2.97	8	7
1:A:11:TRP:HE3	1:A:12:LEU:CD1	0.46	2.23	8	5
1:A:9:ILE:HG23	1:A:12:LEU:HD22	0.46	1.86	1	2
1:A:8:TYR:O	1:A:12:LEU:HG	0.45	2.11	2	1
1:A:19:SER:OG	1:A:21:ARG:HG3	0.44	2.12	3	4
1:A:15:GLY:HA3	1:A:19:SER:HB3	0.44	1.89	3	5
1:A:6:ARG:CG	1:A:7:LEU:H	0.44	2.26	7	1
1:A:8:TYR:CE1	1:A:12:LEU:CD1	0.43	3.00	6	5
1:A:5:VAL:O	1:A:9:ILE:N	0.43	2.45	3	1
1:A:5:VAL:CG1	1:A:9:ILE:CD1	0.42	2.97	2	2
1:A:7:LEU:CD1	1:A:25:CYS:HB2	0.42	2.44	9	1
1:A:7:LEU:O	1:A:24:PRO:HG3	0.42	2.14	10	1
1:A:8:TYR:HB2	1:A:25:CYS:CB	0.42	2.44	5	4
1:A:9:ILE:CA	1:A:12:LEU:HD13	0.42	2.40	9	3
1:A:15:GLY:HA3	1:A:19:SER:CB	0.42	2.45	1	4
1:A:8:TYR:HB2	1:A:25:CYS:HB3	0.42	1.92	9	1
1:A:5:VAL:HA	1:A:8:TYR:CB	0.41	2.46	2	2
1:A:6:ARG:CG	1:A:7:LEU:N	0.41	2.83	7	1
1:A:8:TYR:CE2	1:A:11:TRP:CZ3	0.41	3.08	6	3
1:A:5:VAL:HG12	1:A:9:ILE:HG12	0.41	1.88	3	1
1:A:5:VAL:CA	1:A:8:TYR:HB3	0.41	2.44	5	1
1:A:8:TYR:HE1	1:A:12:LEU:HD11	0.41	1.68	2	1
1:A:11:TRP:CD1	1:A:21:ARG:HB2	0.40	2.50	1	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	20/25 (80%)	19±0 (95±0%)	1±0 (3±2%)	0±0 (2±2%)	8	49
All	All	200/250 (80%)	190 (95%)	6 (3%)	4 (2%)	8	49

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	15	GLY	4

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	18/22 (82%)	16±1 (87±6%)	2±1 (13±6%)	6	46
All	All	180/220 (82%)	156 (87%)	24 (13%)	6	46

All 5 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	9	ILE	7
1	A	10	GLN	7
1	A	7	LEU	4
1	A	6	ARG	3
1	A	21	ARG	3

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 52% for the well-defined parts and 51% for the entire structure.

7.1 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *nef_chemical_shift_list_ShiftList_310K_20160428*

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)	2

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 52%, i.e. 147 atoms were assigned a chemical shift out of a possible 284. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	41/100 (41%)	41/41 (100%)	0/42 (0%)	0/17 (0%)
Sidechain	96/163 (59%)	96/106 (91%)	0/49 (0%)	0/8 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	147/284 (52%)	147/157 (94%)	0/101 (0%)	0/26 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 167 atoms were assigned a chemical shift out of a possible 328. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	47/120 (39%)	47/49 (96%)	0/50 (0%)	0/21 (0%)
Sidechain	110/187 (59%)	110/120 (92%)	0/59 (0%)	0/8 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	167/328 (51%)	167/179 (93%)	0/119 (0%)	0/30 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

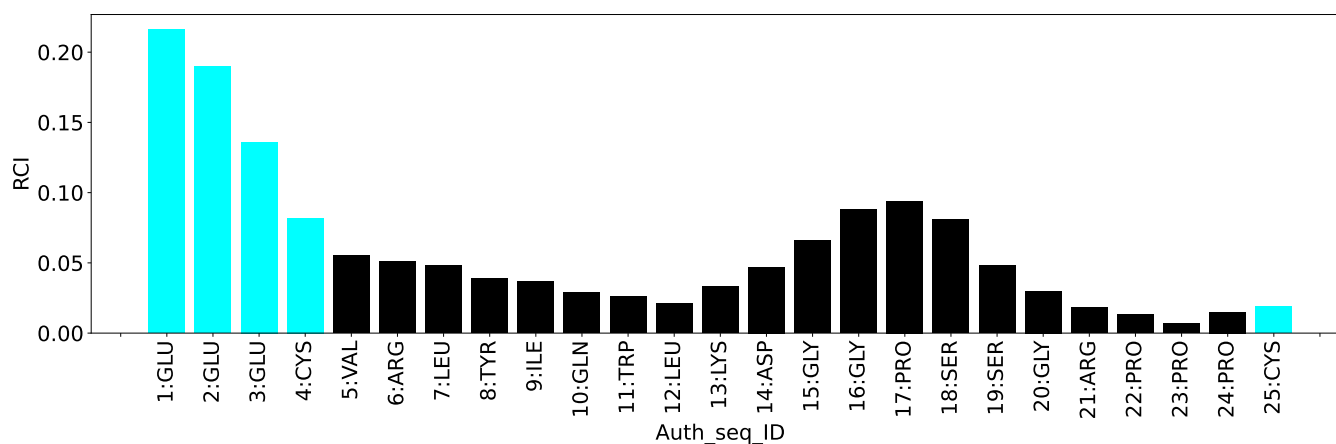
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	16	GLY	HA2	0.74	2.15 – 5.77	-8.9
2	A	23	PRO	HA	2.28	2.78 – 6.00	-6.6

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	2016
Intra-residue ($ i-j =0$)	948
Sequential ($ i-j =1$)	375
Medium range ($ i-j >1$ and $ i-j <5$)	378
Long range ($ i-j \geq 5$)	315
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	80.6
Number of long range restraints per residue ¹	12.6

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)	86.4	0.2
0.2-0.5 (Medium)	169.0	0.5
>0.5 (Large)	180.5	3.88

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

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

9 Distance violation analysis ⓘ

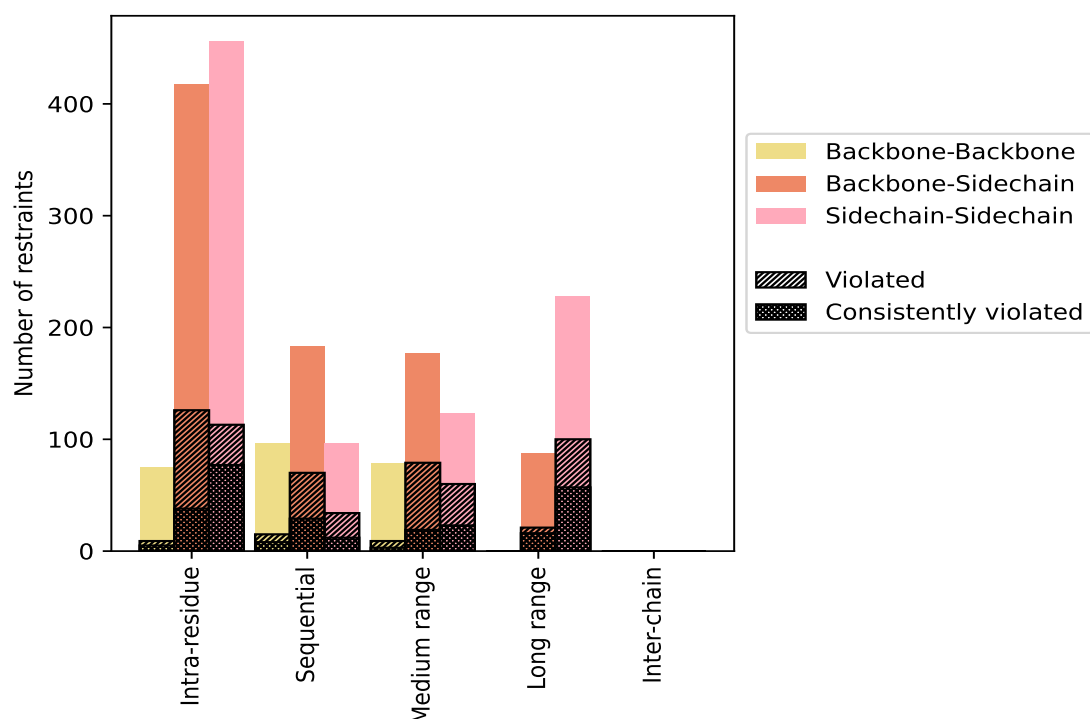
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	948	47.0	248	26.2	12.3	120	12.7	6.0
Backbone-Backbone	75	3.7	9	12.0	0.4	5	6.7	0.2
Backbone-Sidechain	417	20.7	126	30.2	6.2	38	9.1	1.9
Sidechain-Sidechain	456	22.6	113	24.8	5.6	77	16.9	3.8
Sequential ($i-j =1$)	375	18.6	119	31.7	5.9	49	13.1	2.4
Backbone-Backbone	96	4.8	15	15.6	0.7	8	8.3	0.4
Backbone-Sidechain	183	9.1	70	38.3	3.5	29	15.8	1.4
Sidechain-Sidechain	96	4.8	34	35.4	1.7	12	12.5	0.6
Medium range ($i-j >1$ & $i-j <5$)	378	18.8	148	39.2	7.3	45	11.9	2.2
Backbone-Backbone	78	3.9	9	11.5	0.4	3	3.8	0.1
Backbone-Sidechain	177	8.8	79	44.6	3.9	19	10.7	0.9
Sidechain-Sidechain	123	6.1	60	48.8	3.0	23	18.7	1.1
Long range ($i-j \geq 5$)	315	15.6	121	38.4	6.0	73	23.2	3.6
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	87	4.3	21	24.1	1.0	16	18.4	0.8
Sidechain-Sidechain	228	11.3	100	43.9	5.0	57	25.0	2.8
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	2016	100.0	636	31.5	31.5	287	14.2	14.2
Backbone-Backbone	249	12.4	33	13.3	1.6	16	6.4	0.8
Backbone-Sidechain	864	42.9	296	34.3	14.7	102	11.8	5.1
Sidechain-Sidechain	903	44.8	307	34.0	15.2	169	18.7	8.4

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 disulfid bonds are counted in their appropriate category on the x-axis

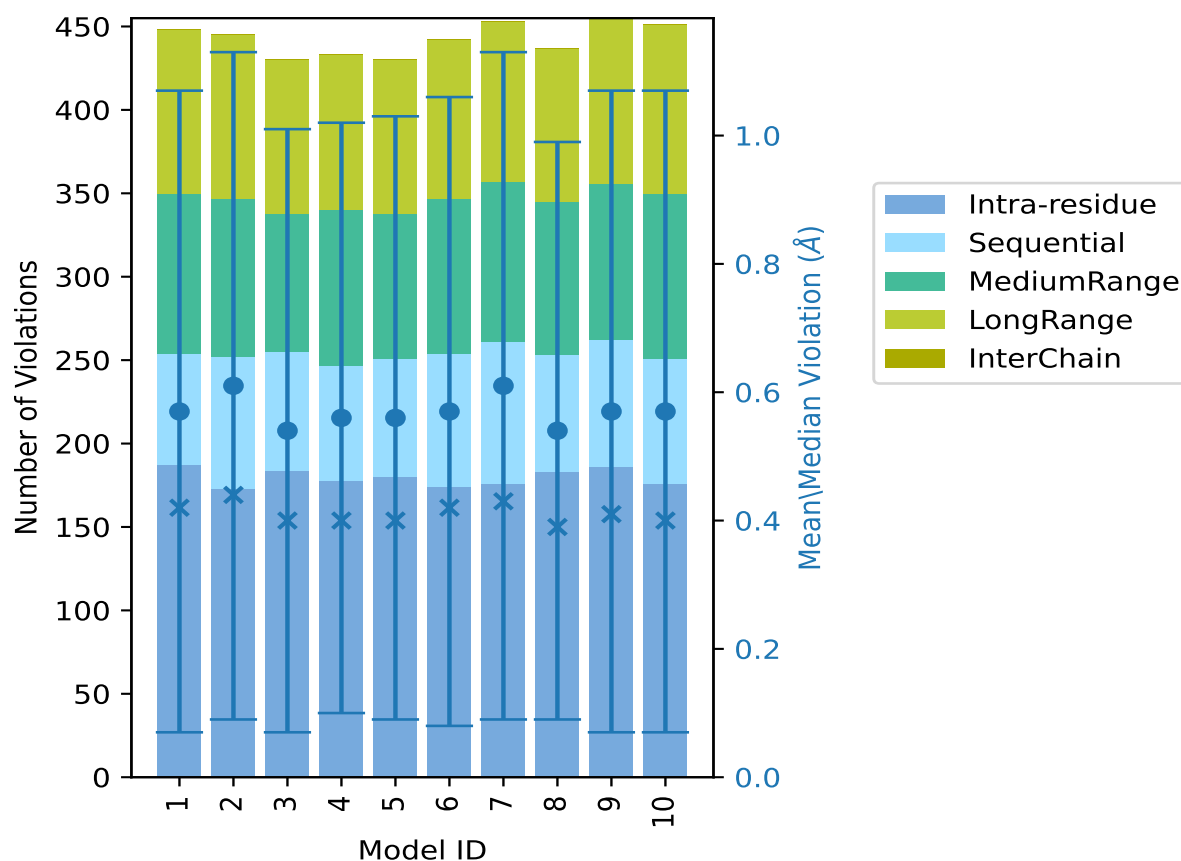
9.2 Distance violation statistics for each model [i](#)

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	187	67	96	98	0	448	0.57	3.8	0.5	0.42
2	173	79	95	98	0	445	0.61	3.28	0.52	0.44
3	184	71	83	92	0	430	0.54	3.28	0.47	0.4
4	178	69	93	93	0	433	0.56	3.27	0.46	0.4
5	180	71	87	92	0	430	0.56	3.28	0.47	0.4
6	174	80	93	95	0	442	0.57	3.28	0.49	0.42
7	176	85	96	96	0	453	0.61	3.82	0.52	0.43
8	183	70	92	92	0	437	0.54	3.28	0.45	0.39
9	186	76	94	99	0	455	0.57	3.88	0.5	0.41
10	176	75	99	101	0	451	0.57	3.28	0.5	0.4

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, 1380(IR:700, SQ:256, MR:230, LR:194, 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	%
13	12	10	13	0	48	1	10.0
25	16	33	7	0	81	2	20.0
15	13	4	0	0	32	3	30.0

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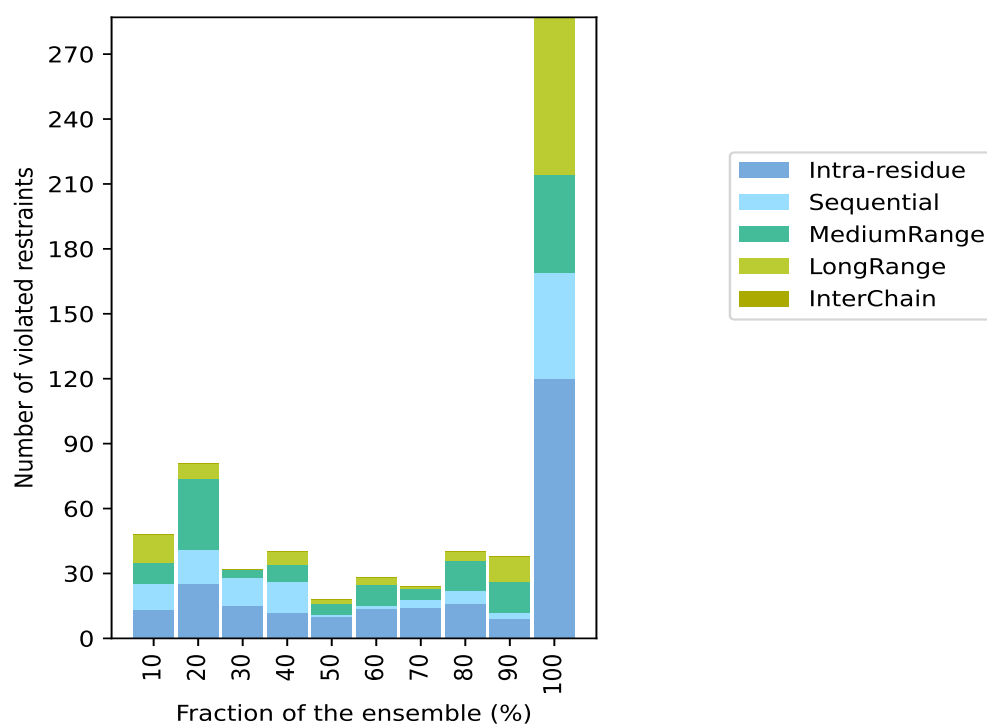
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
12	14	8	6	0	40	4	40.0
10	1	5	2	0	18	5	50.0
14	1	10	3	0	28	6	60.0
14	4	5	1	0	24	7	70.0
16	6	14	4	0	40	8	80.0
9	3	14	12	0	38	9	90.0
120	49	45	73	0	287	10	100.0

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

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

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

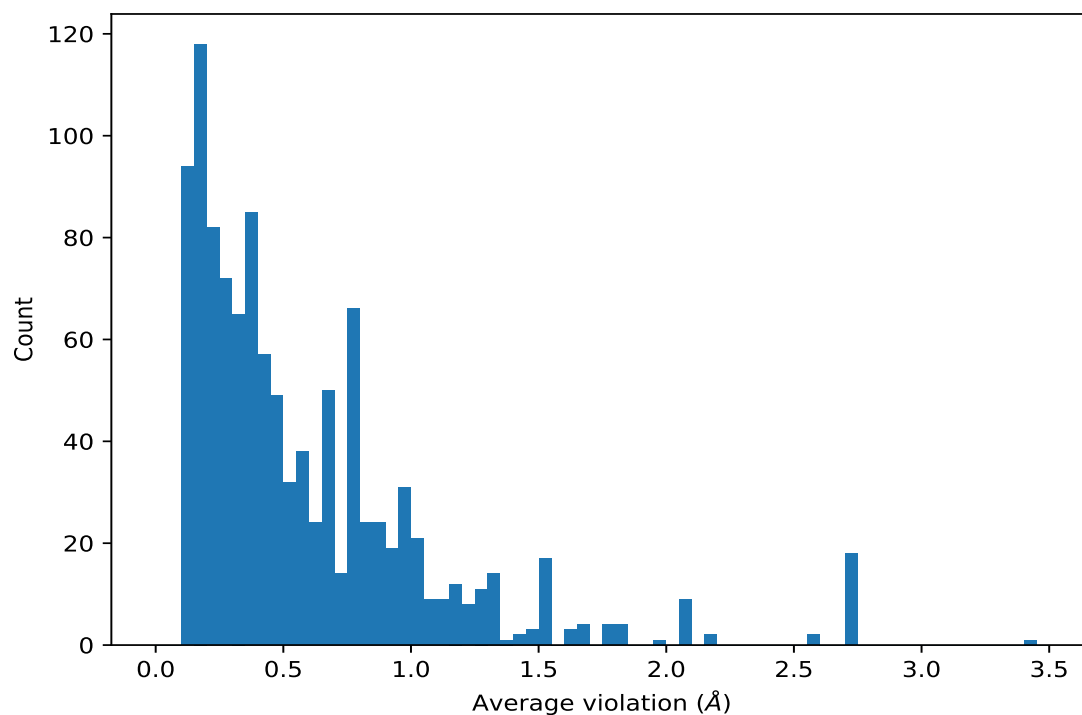


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,669)	1:1:A:GLU:HA	1:1:A:GLU:HB2	10	3.44	0.25	3.28
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	10	2.72	0.28	2.81
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	10	2.72	0.28	2.81
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	10	2.72	0.28	2.81
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	10	2.72	0.28	2.81
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	10	2.72	0.28	2.81
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	10	2.72	0.28	2.81
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	10	2.72	0.28	2.81
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	10	2.72	0.28	2.81
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	10	2.72	0.28	2.81
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	10	2.72	0.28	2.81
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	10	2.72	0.28	2.81
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	10	2.72	0.28	2.81
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	10	2.72	0.28	2.81
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	10	2.72	0.28	2.81

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	10	2.72	0.28	2.81
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	10	2.72	0.28	2.81
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	10	2.72	0.28	2.81
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	10	2.72	0.28	2.81
(2,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	2.58	0.06	2.57
(4,35)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	2.58	0.06	2.57
(2,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	10	2.15	0.44	1.87
(4,42)	1:6:A:ARG:H	1:9:A:ILE:HG12	10	2.15	0.44	1.87
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	10	2.06	0.28	2.16
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	10	2.06	0.28	2.16
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	10	2.06	0.28	2.16
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	10	2.06	0.28	2.16
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	10	2.06	0.28	2.16
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	10	2.06	0.28	2.16
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	10	2.06	0.28	2.16
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	10	2.06	0.28	2.16
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	10	2.06	0.28	2.16
(1,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	1.98	0.06	1.96
(2,101)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.78	0.09	1.73
(4,8)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.78	0.09	1.73
(2,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	10	1.76	0.92	1.18
(3,588)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	10	1.76	0.92	1.18
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	10	1.67	0.03	1.66
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	10	1.67	0.03	1.66
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	10	1.67	0.03	1.66
(2,271)	1:8:A:TYR:H	1:9:A:ILE:HB	10	1.53	0.15	1.53
(4,26)	1:8:A:TYR:H	1:9:A:ILE:HB	10	1.53	0.15	1.53
(1,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	10	1.49	0.44	1.21
(2,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.49	0.01	1.49
(4,15)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.49	0.01	1.49
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	10	1.44	0.09	1.4
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	10	1.44	0.09	1.4
(2,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	1.32	0.02	1.32
(3,144)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	1.32	0.02	1.32
(1,443)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	1.29	0.06	1.27
(2,227)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	10	1.29	0.05	1.29
(3,202)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	10	1.29	0.05	1.29
(1,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	10	1.28	0.02	1.28
(1,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	10	1.28	0.02	1.28
(2,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	10	1.21	0.28	1.27
(4,30)	1:10:A:GLN:HE22	1:11:A:TRP:H	10	1.21	0.28	1.27
(1,122)	1:10:A:GLN:HA	1:10:A:GLN:HE21	10	1.2	0.16	1.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	10	1.19	0.51	0.94
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	10	1.19	0.51	0.94
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	10	1.19	0.51	0.94
(2,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	1.17	0.02	1.18
(4,36)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	1.17	0.02	1.18
(1,101)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.12	0.09	1.07
(1,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	10	1.11	0.92	0.52
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	10	1.1	0.11	1.08
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	10	1.1	0.11	1.08
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	10	1.1	0.11	1.08
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	10	1.1	0.11	1.08
(2,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	10	1.09	0.12	1.06
(3,172)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	10	1.09	0.12	1.06
(1,610)	1:15:A:GLY:HA3	1:19:A:SER:HB3	10	1.06	0.12	1.09
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG2	10	1.06	0.04	1.07
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG3	10	1.06	0.04	1.07
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG2	10	1.05	0.36	0.97
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG3	10	1.05	0.36	0.97
(1,647)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	10	1.02	0.39	1.25
(1,647)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	10	1.02	0.39	1.25
(1,647)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	10	1.02	0.39	1.25
(2,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.02	0.02	1.02
(3,147)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.02	0.02	1.02
(1,665)	1:10:A:GLN:HA	1:13:A:LYS:HD3	10	1.0	0.41	1.02
(1,567)	1:12:A:LEU:HA	1:16:A:GLY:HA2	10	1.0	0.12	0.97
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.98	0.13	0.93
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.98	0.13	0.93
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.98	0.13	0.93
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	10	0.98	0.13	0.93
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	10	0.98	0.13	0.93
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	10	0.98	0.13	0.93
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.98	0.13	0.93
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.98	0.13	0.93
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.98	0.13	0.93
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	10	0.98	0.13	0.93
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	10	0.98	0.13	0.93
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	10	0.98	0.13	0.93
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	10	0.98	0.23	1.1
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	10	0.98	0.23	1.1
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	10	0.98	0.23	1.1
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	10	0.98	0.23	1.1
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	10	0.98	0.23	1.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	10	0.98	0.23	1.1
(1,559)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	10	0.94	0.04	0.94
(1,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	0.94	0.01	0.94
(2,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	10	0.92	0.02	0.92
(3,461)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	10	0.92	0.02	0.92
(2,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	10	0.91	0.13	0.88
(3,148)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	10	0.91	0.13	0.88
(1,536)	1:8:A:TYR:HA	1:24:A:PRO:HG2	10	0.89	0.03	0.89
(1,627)	1:14:A:ASP:HB3	1:19:A:SER:HB2	10	0.89	0.18	0.84
(1,271)	1:8:A:TYR:H	1:9:A:ILE:HB	10	0.88	0.15	0.88
(1,537)	1:8:A:TYR:HA	1:24:A:PRO:HG3	10	0.87	0.04	0.86
(2,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	10	0.87	0.7	0.53
(2,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	10	0.87	0.7	0.53
(2,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	10	0.87	0.7	0.53
(3,594)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	10	0.87	0.7	0.53
(3,594)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	10	0.87	0.7	0.53
(3,594)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	10	0.87	0.7	0.53
(2,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	10	0.86	0.15	0.95
(3,575)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	10	0.86	0.15	0.95
(1,487)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.85	0.01	0.86
(1,472)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	10	0.85	0.06	0.85
(2,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.85	0.07	0.84
(3,145)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.85	0.07	0.84
(1,281)	1:24:A:PRO:HG2	1:25:A:CYS:H	10	0.83	0.15	0.82
(1,568)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	10	0.82	0.05	0.84
(2,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.82	0.05	0.82
(2,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	10	0.82	0.8	0.18
(3,146)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.82	0.05	0.82
(3,587)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	10	0.82	0.8	0.18
(1,244)	1:8:A:TYR:HD1	1:9:A:ILE:H	10	0.82	0.16	0.88
(1,244)	1:8:A:TYR:HD2	1:9:A:ILE:H	10	0.82	0.16	0.88
(1,324)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	10	0.81	0.21	0.76
(1,212)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	10	0.8	0.11	0.78
(1,543)	1:8:A:TYR:HA	1:24:A:PRO:HD2	10	0.8	0.04	0.82
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	10	0.79	0.08	0.8
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	10	0.79	0.08	0.8
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	10	0.79	0.08	0.8
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	10	0.79	0.08	0.8
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	10	0.79	0.08	0.8
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	10	0.79	0.08	0.8
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	10	0.79	0.08	0.8
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	10	0.79	0.08	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	10	0.79	0.08	0.8
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	10	0.79	0.08	0.8
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	10	0.79	0.08	0.8
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	10	0.79	0.08	0.8
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	10	0.79	0.08	0.8
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	10	0.79	0.08	0.8
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	10	0.79	0.08	0.8
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	10	0.79	0.08	0.8
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	10	0.79	0.08	0.8
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	10	0.79	0.08	0.8
(1,628)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	10	0.78	0.1	0.8
(1,498)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	10	0.78	0.06	0.79
(2,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.78	0.05	0.8
(3,489)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.78	0.05	0.8
(1,59)	1:9:A:ILE:H	1:9:A:ILE:HG13	10	0.78	0.03	0.78
(2,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	10	0.78	0.21	0.85
(2,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	10	0.78	0.21	0.85
(4,21)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	10	0.78	0.21	0.85
(4,21)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	10	0.78	0.21	0.85
(2,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.77	0.1	0.78
(3,163)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.77	0.1	0.78
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	0.76	0.01	0.76
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	0.76	0.01	0.76
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	10	0.76	0.01	0.76
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	10	0.76	0.01	0.76
(1,577)	1:20:A:GLY:H	1:21:A:ARG:H	10	0.76	0.2	0.76
(1,588)	1:14:A:ASP:HB3	1:15:A:GLY:H	10	0.75	0.11	0.76
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	10	0.74	0.15	0.75
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	10	0.74	0.15	0.75
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	10	0.74	0.15	0.75
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	10	0.74	0.15	0.75
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	10	0.74	0.15	0.75
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	10	0.74	0.15	0.75
(2,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.74	0.41	0.93
(3,103)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.74	0.41	0.93
(1,447)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.73	0.03	0.71
(2,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	10	0.72	0.18	0.74
(3,550)	1:2:A:GLU:HB2	1:5:A:VAL:H	10	0.72	0.18	0.74
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.7	0.25	0.81
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.7	0.25	0.81
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.7	0.25	0.81
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB2	10	0.7	0.04	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB3	10	0.7	0.04	0.7
(1,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	0.69	0.02	0.69
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	10	0.69	0.04	0.68
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	10	0.69	0.04	0.68
(1,267)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	10	0.68	0.03	0.68
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG2	10	0.68	0.1	0.7
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG3	10	0.68	0.1	0.7
(1,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	10	0.68	0.12	0.65
(1,668)	1:1:A:GLU:HA	1:1:A:GLU:HB3	10	0.68	0.18	0.72
(2,228)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	10	0.66	0.11	0.64
(3,203)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	10	0.66	0.11	0.64
(1,234)	1:14:A:ASP:HB3	1:15:A:GLY:H	10	0.66	0.11	0.66
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	10	0.66	0.27	0.62
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	10	0.66	0.27	0.62
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	10	0.66	0.27	0.62
(1,630)	1:2:A:GLU:HG2	1:5:A:VAL:HB	10	0.66	0.19	0.55
(1,630)	1:2:A:GLU:HG3	1:5:A:VAL:HB	10	0.66	0.19	0.55
(2,604)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.66	0.03	0.66
(2,604)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.66	0.03	0.66
(3,561)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.66	0.03	0.66
(3,561)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.66	0.03	0.66
(1,246)	1:8:A:TYR:HD1	1:25:A:CYS:H	10	0.64	0.12	0.62
(1,246)	1:8:A:TYR:HD2	1:25:A:CYS:H	10	0.64	0.12	0.62
(2,508)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	10	0.63	0.0	0.63
(4,37)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	10	0.63	0.0	0.63
(1,661)	1:9:A:ILE:HA	1:12:A:LEU:HB2	10	0.62	0.09	0.66
(1,153)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	10	0.61	0.05	0.6
(1,403)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.61	0.01	0.62
(1,600)	1:11:A:TRP:HZ3	1:17:A:PRO:HD3	10	0.61	0.13	0.64
(1,467)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.61	0.01	0.61
(1,176)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	10	0.61	0.05	0.61
(1,176)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	10	0.61	0.05	0.61
(1,442)	1:22:A:PRO:HA	1:22:A:PRO:HD3	10	0.6	0.03	0.6
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	10	0.56	0.72	0.21
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	10	0.56	0.72	0.21
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	10	0.56	0.72	0.21
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	10	0.56	0.72	0.21
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	10	0.56	0.72	0.21
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	10	0.56	0.72	0.21
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	10	0.56	0.72	0.21
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	10	0.56	0.72	0.21
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	10	0.56	0.72	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	10	0.56	0.72	0.21
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	10	0.56	0.72	0.21
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	10	0.56	0.72	0.21
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	10	0.56	0.72	0.21
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	10	0.56	0.72	0.21
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	10	0.56	0.72	0.21
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	10	0.56	0.72	0.21
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	10	0.56	0.72	0.21
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	10	0.56	0.72	0.21
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.55	0.1	0.56
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	10	0.55	0.1	0.56
(1,477)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.55	0.02	0.54
(2,419)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	10	0.54	0.01	0.54
(3,385)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	10	0.54	0.01	0.54
(1,501)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.54	0.01	0.54
(2,76)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.54	0.08	0.57
(3,69)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.54	0.08	0.57
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	10	0.53	0.1	0.46
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	10	0.53	0.1	0.46
(2,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	10	0.52	0.19	0.44
(3,171)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	10	0.52	0.19	0.44
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	10	0.52	0.09	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	10	0.52	0.09	0.59
(1,294)	1:2:A:GLU:HA	1:2:A:GLU:HB3	10	0.52	0.08	0.49
(1,446)	1:22:A:PRO:HA	1:22:A:PRO:HG2	10	0.51	0.08	0.55
(1,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	0.51	0.02	0.52
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	10	0.5	0.08	0.52
(2,116)	1:24:A:PRO:HB3	1:25:A:CYS:H	10	0.49	0.04	0.5
(3,107)	1:24:A:PRO:HB3	1:25:A:CYS:H	10	0.49	0.04	0.5
(1,346)	1:9:A:ILE:HA	1:9:A:ILE:HG12	10	0.49	0.08	0.45
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	10	0.48	0.19	0.39
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	10	0.48	0.19	0.39
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	10	0.48	0.19	0.39
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	10	0.48	0.19	0.39
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	10	0.48	0.19	0.39
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	10	0.48	0.19	0.39
(1,462)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	10	0.47	0.01	0.47
(1,326)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	10	0.47	0.04	0.47
(1,430)	1:21:A:ARG:HA	1:21:A:ARG:HB3	10	0.46	0.01	0.46
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	10	0.45	0.13	0.4
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	10	0.45	0.13	0.4
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	10	0.45	0.13	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	10	0.44	0.08	0.44
(3,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	10	0.44	0.08	0.44
(1,455)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.44	0.02	0.45
(2,351)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.43	0.02	0.43
(3,320)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.43	0.02	0.43
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD11	10	0.43	0.06	0.45
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD12	10	0.43	0.06	0.45
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD13	10	0.43	0.06	0.45
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD11	10	0.43	0.06	0.45
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD12	10	0.43	0.06	0.45
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD13	10	0.43	0.06	0.45
(2,52)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.43	0.03	0.44
(3,46)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.43	0.03	0.44
(2,603)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.42	0.01	0.42
(4,43)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.42	0.01	0.42
(2,179)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.42	0.05	0.42
(3,162)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.42	0.05	0.42
(1,453)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.42	0.02	0.43
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	0.42	0.03	0.4
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	0.42	0.03	0.4
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	0.42	0.03	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	0.42	0.03	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	0.42	0.03	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	0.42	0.03	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	0.42	0.03	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	0.42	0.03	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	0.42	0.03	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	0.42	0.03	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	0.42	0.03	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	0.42	0.03	0.4
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG2	10	0.41	0.03	0.4
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG3	10	0.41	0.03	0.4
(2,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.41	0.09	0.4
(3,201)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.41	0.09	0.4
(2,217)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.41	0.03	0.41
(2,217)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.41	0.03	0.41
(3,193)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.41	0.03	0.41
(3,193)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.41	0.03	0.41
(1,597)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	10	0.4	0.1	0.44
(2,132)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.4	0.03	0.39
(4,11)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.4	0.03	0.39
(1,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.39	0.02	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.39	0.03	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.39	0.03	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.39	0.03	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.39	0.03	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.39	0.03	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.39	0.03	0.37
(2,137)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	10	0.39	0.06	0.38
(2,175)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.39	0.03	0.4
(2,175)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.39	0.03	0.4
(3,126)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	10	0.39	0.06	0.38
(4,16)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.39	0.03	0.4
(4,16)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.39	0.03	0.4
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	10	0.38	0.12	0.32
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	10	0.38	0.12	0.32
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	10	0.38	0.12	0.32
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	10	0.38	0.12	0.32
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	10	0.38	0.12	0.32
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	10	0.38	0.12	0.32
(2,280)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.38	0.03	0.4
(2,280)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.38	0.03	0.4
(2,280)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.38	0.03	0.4
(4,29)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.38	0.03	0.4
(4,29)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.38	0.03	0.4
(4,29)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.38	0.03	0.4
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	10	0.37	0.15	0.42
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	10	0.37	0.15	0.42
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	10	0.37	0.15	0.42
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	10	0.37	0.15	0.42
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	10	0.37	0.15	0.42
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	10	0.37	0.15	0.42
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	10	0.37	0.15	0.42
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	10	0.37	0.15	0.42
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	10	0.37	0.15	0.42
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	10	0.37	0.15	0.42
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	10	0.37	0.15	0.42
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	10	0.37	0.15	0.42
(1,458)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.37	0.0	0.37
(1,405)	1:17:A:PRO:HA	1:17:A:PRO:HD3	10	0.37	0.05	0.38
(2,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	10	0.37	0.42	0.15
(4,22)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	10	0.37	0.42	0.15
(1,426)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	10	0.36	0.0	0.36
(1,463)	1:21:A:ARG:HA	1:22:A:PRO:HD3	10	0.36	0.1	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,530)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	10	0.36	0.15	0.26
(3,492)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	10	0.36	0.15	0.26
(1,418)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.36	0.0	0.36
(2,177)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.36	0.03	0.36
(4,17)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.36	0.03	0.36
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	10	0.35	0.0	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	10	0.35	0.0	0.35
(1,339)	1:7:A:LEU:HD11	1:7:A:LEU:HG	10	0.35	0.01	0.35
(1,339)	1:7:A:LEU:HD12	1:7:A:LEU:HG	10	0.35	0.01	0.35
(1,339)	1:7:A:LEU:HD13	1:7:A:LEU:HG	10	0.35	0.01	0.35
(1,339)	1:7:A:LEU:HD21	1:7:A:LEU:HG	10	0.35	0.01	0.35
(1,339)	1:7:A:LEU:HD22	1:7:A:LEU:HG	10	0.35	0.01	0.35
(1,339)	1:7:A:LEU:HD23	1:7:A:LEU:HG	10	0.35	0.01	0.35
(1,488)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.35	0.0	0.35
(1,65)	1:18:A:SER:H	1:18:A:SER:HA	10	0.34	0.02	0.34
(2,108)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.34	0.05	0.36
(3,100)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.34	0.05	0.36
(1,75)	1:19:A:SER:H	1:19:A:SER:HB3	10	0.33	0.14	0.29
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	0.33	0.08	0.29
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	10	0.33	0.08	0.29
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.33	0.13	0.29
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.33	0.13	0.29
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.33	0.13	0.29
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	10	0.33	0.13	0.29
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	10	0.33	0.13	0.29
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	10	0.33	0.13	0.29
(1,599)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	10	0.33	0.08	0.31
(1,599)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	10	0.33	0.08	0.31
(1,372)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.32	0.0	0.32
(1,91)	1:11:A:TRP:HE1	1:19:A:SER:HG	10	0.32	0.07	0.31
(1,476)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.31	0.02	0.31
(1,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	10	0.31	0.13	0.29
(1,268)	1:8:A:TYR:H	1:24:A:PRO:HG2	10	0.31	0.11	0.32
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	10	0.3	0.13	0.26
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	10	0.3	0.13	0.26
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	10	0.3	0.13	0.26
(1,503)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.3	0.02	0.3
(2,125)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.3	0.01	0.3
(4,10)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.3	0.01	0.3
(1,491)	1:24:A:PRO:HA	1:24:A:PRO:HB3	10	0.29	0.01	0.3
(1,529)	1:11:A:TRP:HB3	1:24:A:PRO:HD2	10	0.29	0.07	0.29
(2,169)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.29	0.01	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,14)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.29	0.01	0.29
(1,328)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.29	0.04	0.29
(1,138)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.28	0.06	0.31
(1,138)	1:8:A:TYR:HB3	1:9:A:ILE:H	10	0.28	0.06	0.31
(1,205)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	10	0.28	0.08	0.29
(1,205)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	10	0.28	0.08	0.29
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.28	0.06	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.28	0.06	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.28	0.06	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	10	0.28	0.06	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	10	0.28	0.06	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	10	0.28	0.06	0.24
(1,354)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	10	0.28	0.01	0.28
(1,354)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	10	0.28	0.01	0.28
(1,354)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	10	0.28	0.01	0.28
(1,404)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.27	0.0	0.27
(1,558)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	10	0.27	0.05	0.29
(1,352)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	10	0.27	0.01	0.27
(2,30)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.27	0.06	0.28
(3,26)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.27	0.06	0.28
(1,544)	1:8:A:TYR:HA	1:24:A:PRO:HD3	10	0.27	0.02	0.28
(1,379)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.27	0.0	0.27
(1,552)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.26	0.08	0.24
(1,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.26	0.03	0.26
(1,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	10	0.26	0.02	0.26
(1,425)	1:19:A:SER:HB2	1:19:A:SER:HB3	10	0.26	0.01	0.26
(2,278)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.25	0.1	0.2
(2,278)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.25	0.1	0.2
(2,278)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.25	0.1	0.2
(3,250)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.25	0.1	0.2
(3,250)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.25	0.1	0.2
(3,250)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.25	0.1	0.2
(1,333)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.25	0.01	0.24
(1,400)	1:14:A:ASP:HA	1:14:A:ASP:HB2	10	0.24	0.04	0.25
(1,407)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.23	0.01	0.23
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	10	0.23	0.09	0.26
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	10	0.23	0.09	0.26
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	10	0.23	0.09	0.26
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	10	0.23	0.09	0.26
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	10	0.23	0.09	0.26
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	10	0.23	0.09	0.26
(2,239)	1:15:A:GLY:HA2	1:16:A:GLY:H	10	0.23	0.05	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,214)	1:15:A:GLY:HA2	1:16:A:GLY:H	10	0.23	0.05	0.24
(1,131)	1:9:A:ILE:HA	1:12:A:LEU:H	10	0.23	0.06	0.2
(1,551)	1:22:A:PRO:HA	1:23:A:PRO:HD2	10	0.23	0.04	0.23
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.22	0.01	0.22
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.22	0.01	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.22	0.01	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.22	0.01	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.22	0.01	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.22	0.01	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.22	0.01	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.22	0.01	0.22
(1,459)	1:22:A:PRO:HB3	1:22:A:PRO:HG3	10	0.22	0.01	0.22
(1,80)	1:5:A:VAL:HA	1:8:A:TYR:H	10	0.22	0.05	0.22
(2,15)	1:9:A:ILE:HG21	1:10:A:GLN:H	10	0.22	0.04	0.22
(2,15)	1:9:A:ILE:HG22	1:10:A:GLN:H	10	0.22	0.04	0.22
(2,15)	1:9:A:ILE:HG23	1:10:A:GLN:H	10	0.22	0.04	0.22
(4,4)	1:9:A:ILE:HG21	1:10:A:GLN:H	10	0.22	0.04	0.22
(4,4)	1:9:A:ILE:HG22	1:10:A:GLN:H	10	0.22	0.04	0.22
(4,4)	1:9:A:ILE:HG23	1:10:A:GLN:H	10	0.22	0.04	0.22
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.21	0.02	0.22
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.21	0.02	0.22
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.21	0.02	0.22
(3,600)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.21	0.02	0.22
(3,600)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.21	0.02	0.22
(3,600)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.21	0.02	0.22
(1,145)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	10	0.21	0.06	0.21
(1,469)	1:23:A:PRO:HA	1:23:A:PRO:HD3	10	0.21	0.03	0.22
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.21	0.0	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	10	0.21	0.0	0.21
(1,164)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	0.2	0.01	0.2
(1,381)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.2	0.0	0.2
(1,381)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.2	0.0	0.2
(1,381)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.2	0.0	0.2
(1,410)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.2	0.0	0.2
(1,302)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	10	0.19	0.0	0.19
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.19	0.04	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.19	0.04	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.19	0.04	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.19	0.04	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.19	0.04	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.19	0.04	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.19	0.04	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.19	0.04	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.19	0.04	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.19	0.04	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.19	0.04	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.19	0.04	0.22
(1,402)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	10	0.19	0.0	0.19
(1,504)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	10	0.19	0.0	0.19
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG11	10	0.19	0.04	0.21
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG12	10	0.19	0.04	0.21
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG13	10	0.19	0.04	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG11	10	0.19	0.04	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG12	10	0.19	0.04	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG13	10	0.19	0.04	0.21
(1,371)	1:11:A:TRP:HA	1:11:A:TRP:HB2	10	0.19	0.01	0.19
(1,382)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.19	0.03	0.2
(1,382)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.19	0.03	0.2
(1,382)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.19	0.03	0.2
(1,516)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	10	0.18	0.0	0.18
(1,308)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	10	0.18	0.0	0.18
(2,273)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.18	0.03	0.17
(4,27)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.18	0.03	0.17
(1,672)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	10	0.18	0.0	0.18
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	10	0.17	0.04	0.19
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	10	0.17	0.04	0.19
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	10	0.17	0.04	0.19
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	10	0.17	0.04	0.19
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	10	0.17	0.04	0.19
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	10	0.17	0.04	0.19
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	10	0.17	0.04	0.19
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	10	0.17	0.04	0.19
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	10	0.17	0.04	0.19
(1,569)	1:23:A:PRO:HA	1:24:A:PRO:HD3	10	0.17	0.05	0.16
(1,341)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.17	0.01	0.17
(1,11)	1:16:A:GLY:H	1:16:A:GLY:HA2	10	0.17	0.01	0.17
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB2	10	0.16	0.01	0.16
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB3	10	0.16	0.01	0.16
(1,448)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	10	0.16	0.0	0.16
(1,495)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	10	0.16	0.0	0.16
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	10	0.16	0.02	0.15
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.16	0.02	0.15
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	10	0.16	0.02	0.15
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.16	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	10	0.16	0.03	0.15
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	10	0.16	0.03	0.15
(2,186)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	10	0.15	0.02	0.15
(3,169)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	10	0.15	0.02	0.15
(1,439)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	10	0.15	0.0	0.15
(1,506)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	10	0.15	0.01	0.14
(1,370)	1:11:A:TRP:HA	1:11:A:TRP:HB3	10	0.14	0.0	0.14
(1,566)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	10	0.13	0.0	0.13
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	10	0.12	0.0	0.12
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	10	0.12	0.0	0.12
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	9	0.96	0.44	0.83
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	9	0.96	0.44	0.83
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	9	0.96	0.44	0.83
(2,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	9	0.89	0.07	0.89
(3,509)	1:14:A:ASP:HB2	1:19:A:SER:HB3	9	0.89	0.07	0.89
(1,635)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	9	0.84	0.36	0.91
(1,635)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	9	0.84	0.36	0.91
(1,635)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	9	0.84	0.36	0.91
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	9	0.8	0.46	0.57
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	9	0.8	0.46	0.57
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	9	0.8	0.46	0.57
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	9	0.8	0.46	0.57
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	9	0.8	0.46	0.57
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	9	0.8	0.46	0.57
(1,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	9	0.77	0.12	0.75
(1,319)	1:6:A:ARG:HA	1:6:A:ARG:HG2	9	0.75	0.14	0.83
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	9	0.71	0.28	0.63
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	9	0.71	0.28	0.63
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	9	0.71	0.28	0.63
(2,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	9	0.61	0.16	0.57
(3,185)	1:23:A:PRO:HB3	1:25:A:CYS:H	9	0.61	0.16	0.57
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	9	0.61	0.2	0.68
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	9	0.61	0.2	0.68
(1,115)	1:2:A:GLU:HB3	1:5:A:VAL:H	9	0.59	0.15	0.66
(1,22)	1:13:A:LYS:H	1:13:A:LYS:HD2	9	0.51	0.15	0.47
(1,634)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	9	0.49	0.2	0.51
(1,634)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	9	0.49	0.2	0.51
(1,634)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	9	0.49	0.2	0.51
(1,479)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	9	0.46	0.03	0.46
(1,143)	1:23:A:PRO:HB2	1:25:A:CYS:H	9	0.43	0.13	0.41
(1,182)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	9	0.42	0.08	0.41
(1,182)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	9	0.42	0.08	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	9	0.38	0.22	0.33
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	9	0.38	0.22	0.33
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	9	0.38	0.22	0.33
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	9	0.38	0.22	0.33
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	9	0.38	0.22	0.33
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	9	0.38	0.22	0.33
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	9	0.38	0.22	0.33
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	9	0.38	0.22	0.33
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	9	0.38	0.22	0.33
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	9	0.38	0.22	0.33
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	9	0.38	0.22	0.33
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	9	0.38	0.22	0.33
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	9	0.38	0.22	0.33
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	9	0.38	0.22	0.33
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	9	0.38	0.22	0.33
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	9	0.38	0.22	0.33
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	9	0.38	0.22	0.33
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	9	0.38	0.22	0.33
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.33	0.05	0.34
(3,32)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.33	0.05	0.34
(1,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	9	0.33	0.07	0.32
(1,629)	1:2:A:GLU:HG3	1:5:A:VAL:HB	9	0.33	0.2	0.2
(1,583)	1:6:A:ARG:HB3	1:7:A:LEU:H	9	0.3	0.11	0.28
(1,486)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	9	0.27	0.01	0.27
(2,211)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	9	0.27	0.12	0.28
(3,189)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	9	0.27	0.12	0.28
(1,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	9	0.24	0.05	0.22
(1,471)	1:11:A:TRP:HH2	1:23:A:PRO:HD3	9	0.21	0.02	0.21
(1,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	9	0.21	0.05	0.19
(1,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	9	0.18	0.04	0.19
(1,570)	1:23:A:PRO:HA	1:24:A:PRO:HD2	9	0.16	0.03	0.16
(2,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	9	0.13	0.02	0.13
(3,375)	1:17:A:PRO:HA	1:17:A:PRO:HG2	9	0.13	0.02	0.13
(1,505)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	9	0.13	0.01	0.12
(2,581)	1:5:A:VAL:HG21	1:9:A:ILE:H	9	0.13	0.02	0.13
(2,581)	1:5:A:VAL:HG22	1:9:A:ILE:H	9	0.13	0.02	0.13
(2,581)	1:5:A:VAL:HG23	1:9:A:ILE:H	9	0.13	0.02	0.13
(3,540)	1:5:A:VAL:HG21	1:9:A:ILE:H	9	0.13	0.02	0.13
(3,540)	1:5:A:VAL:HG22	1:9:A:ILE:H	9	0.13	0.02	0.13
(3,540)	1:5:A:VAL:HG23	1:9:A:ILE:H	9	0.13	0.02	0.13
(2,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	1.8	0.05	1.82
(2,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	1.8	0.05	1.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,24)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	1.8	0.05	1.82
(4,24)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	1.8	0.05	1.82
(1,578)	1:19:A:SER:H	1:20:A:GLY:H	8	1.66	0.05	1.66
(1,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	1.14	0.05	1.16
(1,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	1.14	0.05	1.16
(2,110)	1:12:A:LEU:H	1:12:A:LEU:HG	8	1.03	0.07	1.04
(4,9)	1:12:A:LEU:H	1:12:A:LEU:HG	8	1.03	0.07	1.04
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	8	1.01	0.08	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	8	1.01	0.08	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	8	1.01	0.08	1.03
(1,601)	1:8:A:TYR:HD1	1:25:A:CYS:HB3	8	0.95	0.32	0.87
(1,601)	1:8:A:TYR:HD2	1:25:A:CYS:HB3	8	0.95	0.32	0.87
(1,625)	1:8:A:TYR:HB2	1:25:A:CYS:HB3	8	0.94	0.17	0.98
(1,625)	1:8:A:TYR:HB3	1:25:A:CYS:HB3	8	0.94	0.17	0.98
(2,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	8	0.91	0.22	0.99
(2,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	8	0.91	0.22	0.99
(2,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	8	0.91	0.22	0.99
(4,47)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	8	0.91	0.22	0.99
(4,47)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	8	0.91	0.22	0.99
(4,47)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	8	0.91	0.22	0.99
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	8	0.78	0.21	0.74
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	8	0.78	0.21	0.74
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	8	0.78	0.21	0.74
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD21	8	0.76	0.08	0.78
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD22	8	0.76	0.08	0.78
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD23	8	0.76	0.08	0.78
(2,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.69	0.15	0.73
(4,23)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.69	0.15	0.73
(1,374)	1:12:A:LEU:HA	1:12:A:LEU:HG	8	0.52	0.04	0.51
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	8	0.47	0.14	0.53
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	8	0.47	0.14	0.53
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	8	0.47	0.14	0.53
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	8	0.47	0.14	0.53
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	8	0.47	0.14	0.53
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	8	0.47	0.14	0.53
(1,72)	1:25:A:CYS:H	1:25:A:CYS:HB2	8	0.46	0.12	0.48
(1,323)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	8	0.44	0.19	0.5
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG21	8	0.4	0.2	0.4
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG22	8	0.4	0.2	0.4
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG23	8	0.4	0.2	0.4
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG21	8	0.38	0.07	0.38
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG22	8	0.38	0.07	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG23	8	0.38	0.07	0.38
(1,110)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.37	0.07	0.39
(1,43)	1:4:A:CYS:HB3	1:5:A:VAL:H	8	0.34	0.14	0.37
(1,380)	1:12:A:LEU:HB3	1:12:A:LEU:HG	8	0.34	0.02	0.34
(1,33)	1:10:A:GLN:H	1:10:A:GLN:HB2	8	0.33	0.08	0.35
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG21	8	0.33	0.03	0.34
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG22	8	0.33	0.03	0.34
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG23	8	0.33	0.03	0.34
(1,531)	1:11:A:TRP:HB3	1:24:A:PRO:HG3	8	0.32	0.1	0.29
(1,71)	1:25:A:CYS:H	1:25:A:CYS:HB3	8	0.32	0.11	0.36
(1,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	8	0.3	0.08	0.28
(1,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	8	0.3	0.08	0.28
(1,528)	1:11:A:TRP:HB3	1:24:A:PRO:HD3	8	0.27	0.06	0.26
(1,222)	1:8:A:TYR:HE1	1:9:A:ILE:HG12	8	0.27	0.14	0.21
(1,222)	1:8:A:TYR:HE2	1:9:A:ILE:HG12	8	0.27	0.14	0.21
(1,62)	1:20:A:GLY:H	1:20:A:GLY:HA2	8	0.27	0.04	0.26
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	8	0.19	0.04	0.18
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	8	0.19	0.04	0.18
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	8	0.19	0.04	0.18
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	8	0.19	0.04	0.18
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	8	0.19	0.04	0.18
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	8	0.19	0.04	0.18
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	8	0.19	0.04	0.18
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	8	0.19	0.04	0.18
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	8	0.19	0.04	0.18
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	8	0.19	0.04	0.18
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	8	0.19	0.04	0.18
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	8	0.19	0.04	0.18
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	8	0.19	0.04	0.18
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	8	0.19	0.04	0.18
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	8	0.19	0.04	0.18
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	8	0.19	0.04	0.18
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	8	0.19	0.04	0.18
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	8	0.19	0.04	0.18
(1,306)	1:4:A:CYS:HA	1:4:A:CYS:HB2	8	0.18	0.03	0.19
(1,612)	1:15:A:GLY:HA3	1:19:A:SER:HB2	8	0.16	0.01	0.17
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	8	0.16	0.01	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	8	0.16	0.01	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	8	0.16	0.01	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	8	0.16	0.01	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	8	0.16	0.01	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	8	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	0.14	0.01	0.14
(1,261)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	7	1.39	0.04	1.39
(1,433)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	7	0.65	0.04	0.65
(1,580)	1:5:A:VAL:HG11	1:9:A:ILE:H	7	0.63	0.06	0.62
(1,580)	1:5:A:VAL:HG12	1:9:A:ILE:H	7	0.63	0.06	0.62
(1,580)	1:5:A:VAL:HG13	1:9:A:ILE:H	7	0.63	0.06	0.62
(2,45)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	7	0.6	0.01	0.6
(3,39)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	7	0.6	0.01	0.6
(1,64)	1:18:A:SER:H	1:18:A:SER:HB2	7	0.57	0.12	0.62
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	7	0.5	0.17	0.53
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	7	0.5	0.17	0.53
(1,44)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	7	0.49	0.01	0.49
(1,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	7	0.48	0.12	0.45
(1,435)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	7	0.42	0.04	0.43
(2,230)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	7	0.39	0.0	0.39
(3,205)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	7	0.39	0.0	0.39
(1,534)	1:21:A:ARG:HB3	1:22:A:PRO:HD2	7	0.35	0.09	0.39
(1,593)	1:2:A:GLU:HB3	1:6:A:ARG:H	7	0.35	0.12	0.4
(1,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	7	0.3	0.01	0.3
(1,420)	1:18:A:SER:HA	1:18:A:SER:HB2	7	0.24	0.07	0.25
(2,277)	1:5:A:VAL:HG11	1:6:A:ARG:H	7	0.23	0.03	0.23
(2,277)	1:5:A:VAL:HG12	1:6:A:ARG:H	7	0.23	0.03	0.23
(2,277)	1:5:A:VAL:HG13	1:6:A:ARG:H	7	0.23	0.03	0.23
(4,28)	1:5:A:VAL:HG11	1:6:A:ARG:H	7	0.23	0.03	0.23
(4,28)	1:5:A:VAL:HG12	1:6:A:ARG:H	7	0.23	0.03	0.23
(4,28)	1:5:A:VAL:HG13	1:6:A:ARG:H	7	0.23	0.03	0.23
(1,540)	1:7:A:LEU:HA	1:10:A:GLN:HB2	7	0.2	0.06	0.19
(2,461)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	7	0.17	0.01	0.18
(3,427)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	7	0.17	0.01	0.18
(1,87)	1:19:A:SER:H	1:19:A:SER:HG	7	0.17	0.04	0.17
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	7	0.17	0.04	0.15
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG11	7	0.16	0.03	0.15
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG12	7	0.16	0.03	0.15
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG13	7	0.16	0.03	0.15
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	6	0.7	0.15	0.7
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	6	0.7	0.15	0.7
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	6	0.7	0.15	0.7
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	6	0.7	0.15	0.7
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	6	0.7	0.15	0.7
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	6	0.7	0.15	0.7
(2,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	6	0.63	0.28	0.67
(3,567)	1:15:A:GLY:HA3	1:18:A:SER:HB3	6	0.63	0.28	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,421)	1:18:A:SER:HA	1:18:A:SER:HB3	6	0.6	0.05	0.6
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD11	6	0.47	0.03	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD12	6	0.47	0.03	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD13	6	0.47	0.03	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.47	0.03	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.47	0.03	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.47	0.03	0.47
(1,202)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	6	0.47	0.35	0.46
(1,202)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	6	0.47	0.35	0.46
(1,390)	1:13:A:LYS:HA	1:13:A:LYS:HD2	6	0.46	0.2	0.38
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB2	6	0.45	0.18	0.4
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB3	6	0.45	0.18	0.4
(1,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	6	0.43	0.07	0.42
(1,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	6	0.43	0.07	0.42
(1,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	6	0.43	0.07	0.42
(1,360)	1:10:A:GLN:HA	1:10:A:GLN:HG3	6	0.36	0.13	0.38
(1,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	6	0.36	0.02	0.36
(1,592)	1:2:A:GLU:HB2	1:6:A:ARG:H	6	0.3	0.15	0.23
(1,336)	1:7:A:LEU:HA	1:7:A:LEU:HB3	6	0.28	0.13	0.34
(1,27)	1:4:A:CYS:H	1:4:A:CYS:HB3	6	0.26	0.06	0.26
(1,297)	1:2:A:GLU:HA	1:2:A:GLU:HG2	6	0.22	0.04	0.22
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE2	6	0.22	0.08	0.24
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE3	6	0.22	0.08	0.24
(1,258)	1:14:A:ASP:HB3	1:16:A:GLY:H	6	0.21	0.06	0.24
(1,41)	1:14:A:ASP:H	1:14:A:ASP:HB2	6	0.19	0.04	0.2
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	6	0.19	0.04	0.2
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	6	0.19	0.04	0.2
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	6	0.19	0.04	0.2
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	6	0.19	0.04	0.2
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	6	0.19	0.04	0.2
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	6	0.19	0.04	0.2
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	6	0.19	0.04	0.2
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	6	0.19	0.04	0.2
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	6	0.19	0.04	0.2
(2,219)	1:8:A:TYR:HE1	1:12:A:LEU:HG	6	0.15	0.06	0.13
(2,219)	1:8:A:TYR:HE2	1:12:A:LEU:HG	6	0.15	0.06	0.13
(3,195)	1:8:A:TYR:HE1	1:12:A:LEU:HG	6	0.15	0.06	0.13
(3,195)	1:8:A:TYR:HE2	1:12:A:LEU:HG	6	0.15	0.06	0.13
(1,366)	1:10:A:GLN:HB3	1:10:A:GLN:HG3	6	0.14	0.01	0.14
(2,465)	1:23:A:PRO:HA	1:23:A:PRO:HG2	6	0.13	0.05	0.11
(3,431)	1:23:A:PRO:HA	1:23:A:PRO:HG2	6	0.13	0.05	0.11
(2,266)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	6	0.12	0.03	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,241)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	6	0.12	0.03	0.12
(2,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	6	0.11	0.01	0.12
(3,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	6	0.11	0.01	0.12
(1,314)	1:6:A:ARG:HA	1:6:A:ARG:HD3	5	0.97	0.08	0.97
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD11	5	0.77	0.32	0.93
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD12	5	0.77	0.32	0.93
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD13	5	0.77	0.32	0.93
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD21	5	0.77	0.32	0.93
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD22	5	0.77	0.32	0.93
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD23	5	0.77	0.32	0.93
(2,623)	1:5:A:VAL:HA	1:25:A:CYS:HB2	5	0.59	0.59	0.12
(3,578)	1:5:A:VAL:HA	1:25:A:CYS:HB2	5	0.59	0.59	0.12
(1,322)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	5	0.5	0.11	0.47
(2,17)	1:6:A:ARG:H	1:6:A:ARG:HG3	5	0.47	0.03	0.48
(3,13)	1:6:A:ARG:H	1:6:A:ARG:HG3	5	0.47	0.03	0.48
(2,330)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	5	0.23	0.01	0.23
(3,299)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	5	0.23	0.01	0.23
(1,255)	1:2:A:GLU:HA	1:3:A:GLU:H	5	0.18	0.05	0.21
(2,223)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	5	0.18	0.05	0.17
(2,223)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	5	0.18	0.05	0.17
(3,198)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	5	0.18	0.05	0.17
(3,198)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	5	0.18	0.05	0.17
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB2	5	0.17	0.03	0.17
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB3	5	0.17	0.03	0.17
(1,576)	1:10:A:GLN:H	1:12:A:LEU:H	5	0.12	0.03	0.11
(2,140)	1:7:A:LEU:H	1:7:A:LEU:HB3	5	0.12	0.01	0.12
(3,129)	1:7:A:LEU:H	1:7:A:LEU:HB3	5	0.12	0.01	0.12
(2,347)	1:9:A:ILE:HA	1:9:A:ILE:HG13	5	0.11	0.01	0.1
(3,316)	1:9:A:ILE:HA	1:9:A:ILE:HG13	5	0.11	0.01	0.1
(2,631)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	4	1.54	0.11	1.6
(3,586)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	4	1.54	0.11	1.6
(1,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	4	1.14	0.03	1.14
(2,541)	1:4:A:CYS:HA	1:7:A:LEU:HB2	4	1.06	0.14	1.0
(3,503)	1:4:A:CYS:HA	1:7:A:LEU:HB2	4	1.06	0.14	1.0
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	4	1.02	0.91	1.02
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	4	1.02	0.91	1.02
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	4	1.02	0.91	1.02
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	4	1.02	0.91	1.02
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	4	1.02	0.91	1.02
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	4	1.02	0.91	1.02
(1,631)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	4	0.89	0.11	0.94
(2,104)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.75	0.06	0.78

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,96)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.75	0.06	0.78
(1,269)	1:7:A:LEU:HG	1:8:A:TYR:H	4	0.7	0.07	0.72
(2,662)	1:6:A:ARG:HA	1:9:A:ILE:HG12	4	0.66	0.33	0.81
(3,611)	1:6:A:ARG:HA	1:9:A:ILE:HG12	4	0.66	0.33	0.81
(1,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	4	0.53	0.16	0.45
(1,63)	1:18:A:SER:H	1:18:A:SER:HB3	4	0.53	0.1	0.57
(1,318)	1:6:A:ARG:HA	1:6:A:ARG:HG3	4	0.51	0.05	0.51
(1,541)	1:4:A:CYS:HA	1:7:A:LEU:HB2	4	0.42	0.14	0.36
(2,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	4	0.38	0.01	0.38
(3,480)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	4	0.38	0.01	0.38
(1,26)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.36	0.22	0.34
(1,26)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.36	0.22	0.34
(1,334)	1:7:A:LEU:HA	1:7:A:LEU:HB2	4	0.33	0.08	0.38
(1,564)	1:11:A:TRP:HA	1:14:A:ASP:HB2	4	0.26	0.11	0.24
(1,105)	1:7:A:LEU:H	1:7:A:LEU:HG	4	0.24	0.04	0.24
(2,12)	1:12:A:LEU:HD21	1:13:A:LYS:H	4	0.24	0.1	0.25
(2,12)	1:12:A:LEU:HD22	1:13:A:LYS:H	4	0.24	0.1	0.25
(2,12)	1:12:A:LEU:HD23	1:13:A:LYS:H	4	0.24	0.1	0.25
(4,3)	1:12:A:LEU:HD21	1:13:A:LYS:H	4	0.24	0.1	0.25
(4,3)	1:12:A:LEU:HD22	1:13:A:LYS:H	4	0.24	0.1	0.25
(4,3)	1:12:A:LEU:HD23	1:13:A:LYS:H	4	0.24	0.1	0.25
(2,18)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.23	0.02	0.22
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.23	0.02	0.22
(2,106)	1:6:A:ARG:HG3	1:7:A:LEU:H	4	0.22	0.12	0.16
(2,256)	1:10:A:GLN:HG2	1:11:A:TRP:H	4	0.22	0.03	0.22
(3,98)	1:6:A:ARG:HG3	1:7:A:LEU:H	4	0.22	0.12	0.16
(3,231)	1:10:A:GLN:HG2	1:11:A:TRP:H	4	0.22	0.03	0.22
(1,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	4	0.21	0.1	0.19
(1,304)	1:3:A:GLU:HA	1:3:A:GLU:HB2	4	0.2	0.06	0.2
(1,304)	1:3:A:GLU:HA	1:3:A:GLU:HB3	4	0.2	0.06	0.2
(2,1)	1:7:A:LEU:HB3	1:8:A:TYR:H	4	0.19	0.01	0.19
(3,1)	1:7:A:LEU:HB3	1:8:A:TYR:H	4	0.19	0.01	0.19
(1,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	0.15	0.07	0.12
(2,32)	1:10:A:GLN:H	1:10:A:GLN:HB3	4	0.15	0.06	0.12
(3,27)	1:10:A:GLN:H	1:10:A:GLN:HB3	4	0.15	0.06	0.12
(2,117)	1:24:A:PRO:HG3	1:25:A:CYS:H	4	0.14	0.04	0.13
(3,108)	1:24:A:PRO:HG3	1:25:A:CYS:H	4	0.14	0.04	0.13
(2,270)	1:8:A:TYR:H	1:9:A:ILE:HG12	3	0.5	0.04	0.47
(3,245)	1:8:A:TYR:H	1:9:A:ILE:HG12	3	0.5	0.04	0.47
(1,9)	1:7:A:LEU:HD11	1:8:A:TYR:H	3	0.49	0.12	0.57
(1,9)	1:7:A:LEU:HD12	1:8:A:TYR:H	3	0.49	0.12	0.57
(1,9)	1:7:A:LEU:HD13	1:8:A:TYR:H	3	0.49	0.12	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,9)	1:7:A:LEU:HD21	1:8:A:TYR:H	3	0.49	0.12	0.57
(1,9)	1:7:A:LEU:HD22	1:8:A:TYR:H	3	0.49	0.12	0.57
(1,9)	1:7:A:LEU:HD23	1:8:A:TYR:H	3	0.49	0.12	0.57
(2,369)	1:9:A:ILE:HG12	1:10:A:GLN:H	3	0.4	0.01	0.4
(3,337)	1:9:A:ILE:HG12	1:10:A:GLN:H	3	0.4	0.01	0.4
(1,449)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	3	0.39	0.03	0.39
(1,50)	1:21:A:ARG:H	1:21:A:ARG:HD3	3	0.38	0.02	0.39
(1,538)	1:7:A:LEU:HA	1:10:A:GLN:HB3	3	0.38	0.07	0.37
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.34	0.01	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.34	0.01	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.34	0.01	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.34	0.01	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.34	0.01	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.34	0.01	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.34	0.01	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.34	0.01	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.34	0.01	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.34	0.01	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.34	0.01	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.34	0.01	0.35
(1,662)	1:6:A:ARG:HA	1:9:A:ILE:HG12	3	0.3	0.07	0.3
(2,616)	1:17:A:PRO:HB2	1:18:A:SER:HB2	3	0.29	0.16	0.18
(3,572)	1:17:A:PRO:HB2	1:18:A:SER:HB2	3	0.29	0.16	0.18
(1,445)	1:22:A:PRO:HA	1:22:A:PRO:HG3	3	0.28	0.04	0.28
(1,303)	1:3:A:GLU:HA	1:3:A:GLU:HG2	3	0.25	0.03	0.24
(1,303)	1:3:A:GLU:HA	1:3:A:GLU:HG3	3	0.25	0.03	0.24
(1,28)	1:4:A:CYS:H	1:4:A:CYS:HB2	3	0.24	0.14	0.14
(1,362)	1:10:A:GLN:HA	1:10:A:GLN:HB2	3	0.21	0.02	0.21
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG21	3	0.17	0.02	0.17
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG22	3	0.17	0.02	0.17
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG23	3	0.17	0.02	0.17
(1,150)	1:8:A:TYR:HD1	1:9:A:ILE:HA	3	0.15	0.02	0.16
(1,150)	1:8:A:TYR:HD2	1:9:A:ILE:HA	3	0.15	0.02	0.16
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	3	0.14	0.02	0.15
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	3	0.14	0.02	0.15
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	3	0.14	0.02	0.15
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD11	3	0.14	0.02	0.15
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD12	3	0.14	0.02	0.15
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD13	3	0.14	0.02	0.15
(1,590)	1:24:A:PRO:HB2	1:25:A:CYS:H	3	0.13	0.02	0.14
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	3	0.13	0.01	0.12
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	3	0.13	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	3	0.13	0.01	0.12
(2,31)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.13	0.02	0.12
(4,5)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.13	0.02	0.12
(1,104)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.12	0.0	0.12
(2,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	3	0.12	0.01	0.11
(2,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	3	0.12	0.01	0.11
(3,197)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	3	0.12	0.01	0.11
(3,197)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	3	0.12	0.01	0.11
(1,436)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	3	0.11	0.01	0.11
(1,456)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	3	0.11	0.0	0.11
(2,389)	1:12:A:LEU:HG	1:13:A:LYS:H	3	0.11	0.0	0.11
(3,356)	1:12:A:LEU:HG	1:13:A:LYS:H	3	0.11	0.0	0.11
(1,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	2	1.61	0.05	1.61
(1,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	2	1.61	0.05	1.61
(1,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	2	1.61	0.05	1.61
(2,525)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	2	1.52	0.06	1.52
(2,525)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	2	1.52	0.06	1.52
(2,525)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	2	1.52	0.06	1.52
(4,38)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	2	1.52	0.06	1.52
(4,38)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	2	1.52	0.06	1.52
(4,38)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	2	1.52	0.06	1.52
(1,532)	1:9:A:ILE:HA	1:12:A:LEU:HG	2	1.51	0.01	1.51
(2,287)	1:12:A:LEU:HD11	1:16:A:GLY:H	2	1.5	0.04	1.5
(2,287)	1:12:A:LEU:HD12	1:16:A:GLY:H	2	1.5	0.04	1.5
(2,287)	1:12:A:LEU:HD13	1:16:A:GLY:H	2	1.5	0.04	1.5
(3,258)	1:12:A:LEU:HD11	1:16:A:GLY:H	2	1.5	0.04	1.5
(3,258)	1:12:A:LEU:HD12	1:16:A:GLY:H	2	1.5	0.04	1.5
(3,258)	1:12:A:LEU:HD13	1:16:A:GLY:H	2	1.5	0.04	1.5
(1,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	2	1.34	0.02	1.34
(1,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	2	1.34	0.02	1.34
(1,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	2	1.34	0.02	1.34
(1,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	2	1.34	0.02	1.34
(1,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	2	1.34	0.02	1.34
(1,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	2	1.34	0.02	1.34
(1,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	2	1.34	0.02	1.34
(1,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	2	1.34	0.02	1.34
(1,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	2	1.34	0.02	1.34
(1,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	2	1.34	0.01	1.34
(1,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	2	1.34	0.01	1.34
(1,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	2	1.34	0.01	1.34
(2,377)	1:12:A:LEU:HA	1:12:A:LEU:HD11	2	1.25	0.01	1.25
(2,377)	1:12:A:LEU:HA	1:12:A:LEU:HD12	2	1.25	0.01	1.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,377)	1:12:A:LEU:HA	1:12:A:LEU:HD13	2	1.25	0.01	1.25
(3,345)	1:12:A:LEU:HA	1:12:A:LEU:HD11	2	1.25	0.01	1.25
(3,345)	1:12:A:LEU:HA	1:12:A:LEU:HD12	2	1.25	0.01	1.25
(3,345)	1:12:A:LEU:HA	1:12:A:LEU:HD13	2	1.25	0.01	1.25
(2,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	2	1.21	0.03	1.21
(2,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	2	1.21	0.03	1.21
(2,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	2	1.21	0.03	1.21
(3,173)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	2	1.21	0.03	1.21
(3,173)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	2	1.21	0.03	1.21
(3,173)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	2	1.21	0.03	1.21
(1,376)	1:12:A:LEU:HA	1:12:A:LEU:HD21	2	1.16	0.01	1.16
(1,376)	1:12:A:LEU:HA	1:12:A:LEU:HD22	2	1.16	0.01	1.16
(1,376)	1:12:A:LEU:HA	1:12:A:LEU:HD23	2	1.16	0.01	1.16
(1,198)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	2	1.16	0.03	1.16
(1,198)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	2	1.16	0.03	1.16
(1,198)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	2	1.16	0.03	1.16
(1,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	2	1.0	0.01	1.0
(1,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	2	1.0	0.01	1.0
(1,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	2	1.0	0.01	1.0
(2,10)	1:9:A:ILE:H	1:12:A:LEU:HD21	2	0.98	0.02	0.98
(2,10)	1:9:A:ILE:H	1:12:A:LEU:HD22	2	0.98	0.02	0.98
(2,10)	1:9:A:ILE:H	1:12:A:LEU:HD23	2	0.98	0.02	0.98
(3,8)	1:9:A:ILE:H	1:12:A:LEU:HD21	2	0.98	0.02	0.98
(3,8)	1:9:A:ILE:H	1:12:A:LEU:HD22	2	0.98	0.02	0.98
(3,8)	1:9:A:ILE:H	1:12:A:LEU:HD23	2	0.98	0.02	0.98
(1,287)	1:12:A:LEU:HD11	1:16:A:GLY:H	2	0.96	0.03	0.96
(1,287)	1:12:A:LEU:HD12	1:16:A:GLY:H	2	0.96	0.03	0.96
(1,287)	1:12:A:LEU:HD13	1:16:A:GLY:H	2	0.96	0.03	0.96
(1,658)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	2	0.92	0.28	0.92
(1,658)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	2	0.92	0.28	0.92
(1,658)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	2	0.92	0.28	0.92
(1,525)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	2	0.88	0.05	0.88
(1,525)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	2	0.88	0.05	0.88
(1,525)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	2	0.88	0.05	0.88
(2,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.86	0.02	0.86
(2,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.86	0.02	0.86
(2,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.86	0.02	0.86
(3,175)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.86	0.02	0.86
(3,175)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.86	0.02	0.86
(3,175)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.86	0.02	0.86
(1,194)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	2	0.76	0.01	0.76
(1,194)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	2	0.76	0.01	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,194)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	2	0.76	0.01	0.76
(1,194)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	2	0.76	0.01	0.76
(1,194)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	2	0.76	0.01	0.76
(1,194)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	2	0.76	0.01	0.76
(1,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	2	0.75	0.0	0.75
(1,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	2	0.75	0.0	0.75
(1,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	2	0.75	0.0	0.75
(1,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	2	0.75	0.0	0.75
(1,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	2	0.75	0.0	0.75
(1,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	2	0.75	0.0	0.75
(1,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	2	0.75	0.0	0.75
(1,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	2	0.75	0.0	0.75
(1,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	2	0.75	0.0	0.75
(2,197)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	2	0.68	0.0	0.68
(2,197)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	2	0.68	0.0	0.68
(2,197)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	2	0.68	0.0	0.68
(2,197)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	2	0.68	0.0	0.68
(2,197)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	2	0.68	0.0	0.68
(2,197)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	2	0.68	0.0	0.68
(3,178)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	2	0.68	0.0	0.68
(3,178)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	2	0.68	0.0	0.68
(3,178)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	2	0.68	0.0	0.68
(3,178)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	2	0.68	0.0	0.68
(3,178)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	2	0.68	0.0	0.68
(3,178)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	2	0.68	0.0	0.68
(1,623)	1:5:A:VAL:HA	1:25:A:CYS:HB2	2	0.66	0.08	0.66
(1,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	2	0.61	0.05	0.61
(1,199)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	2	0.61	0.01	0.61
(1,199)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	2	0.61	0.01	0.61
(1,199)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	2	0.61	0.01	0.61
(1,377)	1:12:A:LEU:HA	1:12:A:LEU:HD11	2	0.6	0.01	0.6
(1,377)	1:12:A:LEU:HA	1:12:A:LEU:HD12	2	0.6	0.01	0.6
(1,377)	1:12:A:LEU:HA	1:12:A:LEU:HD13	2	0.6	0.01	0.6
(2,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	2	0.55	0.44	0.55
(2,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	2	0.55	0.44	0.55
(2,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	2	0.55	0.44	0.55
(3,481)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	2	0.55	0.44	0.55
(3,481)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	2	0.55	0.44	0.55
(3,481)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	2	0.55	0.44	0.55
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD11	2	0.52	0.39	0.52
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD12	2	0.52	0.39	0.52
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD13	2	0.52	0.39	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD21	2	0.52	0.39	0.52
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD22	2	0.52	0.39	0.52
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD23	2	0.52	0.39	0.52
(1,361)	1:10:A:GLN:HA	1:10:A:GLN:HG2	2	0.5	0.06	0.5
(2,539)	1:3:A:GLU:HA	1:6:A:ARG:HB3	2	0.46	0.1	0.46
(3,501)	1:3:A:GLU:HA	1:6:A:ARG:HB3	2	0.46	0.1	0.46
(2,664)	1:10:A:GLN:HA	1:13:A:LYS:HD2	2	0.4	0.24	0.4
(3,613)	1:10:A:GLN:HA	1:13:A:LYS:HD2	2	0.4	0.24	0.4
(1,10)	1:9:A:ILE:H	1:12:A:LEU:HD21	2	0.38	0.02	0.38
(1,10)	1:9:A:ILE:H	1:12:A:LEU:HD22	2	0.38	0.02	0.38
(1,10)	1:9:A:ILE:H	1:12:A:LEU:HD23	2	0.38	0.02	0.38
(1,664)	1:10:A:GLN:HA	1:13:A:LYS:HD2	2	0.36	0.19	0.36
(2,25)	1:2:A:GLU:HB2	1:3:A:GLU:H	2	0.34	0.16	0.34
(3,21)	1:2:A:GLU:HB2	1:3:A:GLU:H	2	0.34	0.16	0.34
(2,383)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	2	0.34	0.0	0.34
(2,383)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	2	0.34	0.0	0.34
(2,383)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	2	0.34	0.0	0.34
(3,351)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	2	0.34	0.0	0.34
(3,351)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	2	0.34	0.0	0.34
(3,351)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	2	0.34	0.0	0.34
(1,618)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	2	0.32	0.02	0.32
(1,134)	1:19:A:SER:HB2	1:21:A:ARG:H	2	0.32	0.04	0.32
(1,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	2	0.3	0.04	0.3
(2,394)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	2	0.3	0.05	0.3
(3,361)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	2	0.3	0.05	0.3
(2,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	2	0.29	0.0	0.29
(2,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	2	0.29	0.0	0.29
(2,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	2	0.29	0.0	0.29
(3,602)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	2	0.29	0.0	0.29
(3,602)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	2	0.29	0.0	0.29
(3,602)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	2	0.29	0.0	0.29
(1,102)	1:10:A:GLN:HB3	1:11:A:TRP:H	2	0.24	0.08	0.24
(1,288)	1:12:A:LEU:HA	1:16:A:GLY:H	2	0.22	0.11	0.22
(1,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	2	0.21	0.03	0.21
(1,550)	1:8:A:TYR:HA	1:11:A:TRP:HB3	2	0.2	0.08	0.2
(1,81)	1:4:A:CYS:HA	1:7:A:LEU:H	2	0.19	0.06	0.19
(1,61)	1:20:A:GLY:H	1:20:A:GLY:HA3	2	0.16	0.01	0.16
(2,26)	1:3:A:GLU:H	1:3:A:GLU:HG2	2	0.16	0.02	0.16
(2,26)	1:3:A:GLU:H	1:3:A:GLU:HG3	2	0.16	0.02	0.16
(3,22)	1:3:A:GLU:H	1:3:A:GLU:HG2	2	0.16	0.02	0.16
(3,22)	1:3:A:GLU:H	1:3:A:GLU:HG3	2	0.16	0.02	0.16
(1,385)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	2	0.16	0.01	0.16

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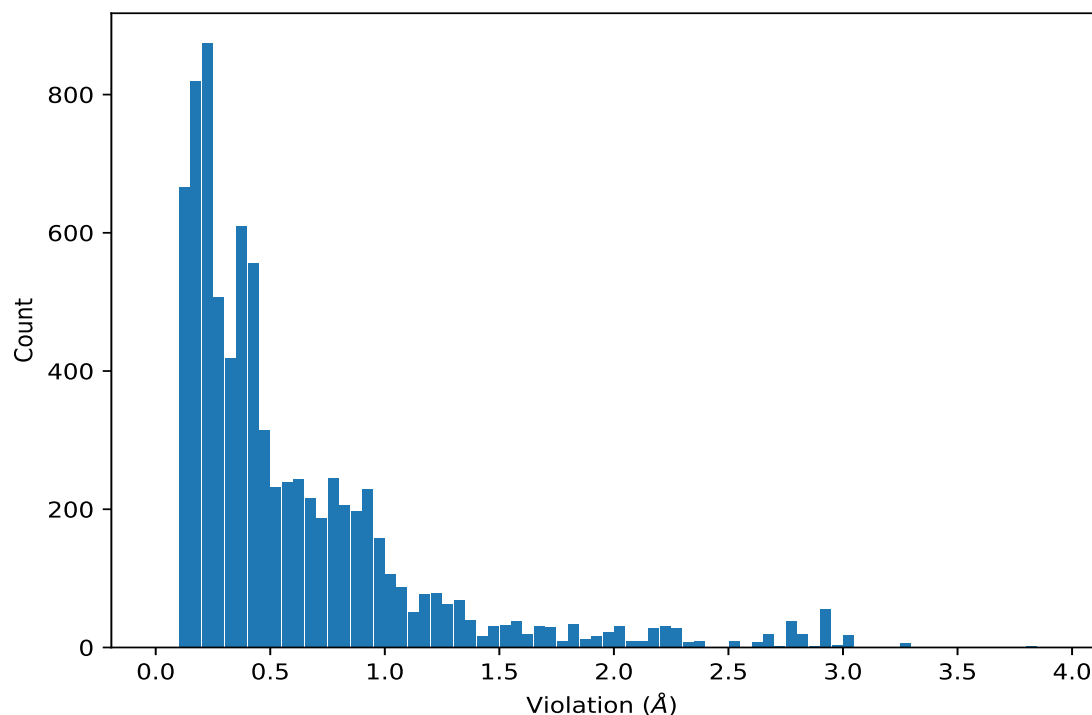
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,385)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	2	0.16	0.01	0.16
(1,385)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	2	0.16	0.01	0.16
(2,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	2	0.15	0.03	0.15
(3,99)	1:9:A:ILE:H	1:9:A:ILE:HG12	2	0.15	0.03	0.15
(1,127)	1:20:A:GLY:HA3	1:21:A:ARG:H	2	0.15	0.02	0.15
(2,152)	1:11:A:TRP:HD1	1:19:A:SER:HB3	2	0.14	0.04	0.14
(3,141)	1:11:A:TRP:HD1	1:19:A:SER:HB3	2	0.14	0.04	0.14
(1,589)	1:23:A:PRO:HA	1:25:A:CYS:H	2	0.13	0.01	0.13
(1,86)	1:18:A:SER:HA	1:19:A:SER:H	2	0.12	0.02	0.12
(1,99)	1:14:A:ASP:H	1:15:A:GLY:H	2	0.12	0.01	0.12
(2,133)	1:8:A:TYR:HA	1:12:A:LEU:H	2	0.12	0.01	0.12
(3,122)	1:8:A:TYR:HA	1:12:A:LEU:H	2	0.12	0.01	0.12
(1,109)	1:12:A:LEU:H	1:12:A:LEU:HB2	2	0.12	0.02	0.12
(1,45)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	2	0.12	0.0	0.12
(2,353)	1:9:A:ILE:HB	1:9:A:ILE:HG13	2	0.12	0.02	0.12
(4,32)	1:9:A:ILE:HB	1:9:A:ILE:HG13	2	0.12	0.02	0.12
(1,395)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	2	0.12	0.0	0.12
(1,395)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	2	0.12	0.0	0.12
(1,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	2	0.12	0.0	0.12
(1,408)	1:17:A:PRO:HA	1:17:A:PRO:HG3	2	0.12	0.0	0.12
(1,670)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	2	0.11	0.0	0.11
(1,670)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	2	0.11	0.0	0.11
(2,556)	1:9:A:ILE:HG21	1:10:A:GLN:HA	2	0.11	0.0	0.11
(2,556)	1:9:A:ILE:HG22	1:10:A:GLN:HA	2	0.11	0.0	0.11
(2,556)	1:9:A:ILE:HG23	1:10:A:GLN:HA	2	0.11	0.0	0.11
(3,518)	1:9:A:ILE:HG21	1:10:A:GLN:HA	2	0.11	0.0	0.11
(3,518)	1:9:A:ILE:HG22	1:10:A:GLN:HA	2	0.11	0.0	0.11
(3,518)	1:9:A:ILE:HG23	1:10:A:GLN:HA	2	0.11	0.0	0.11
(2,272)	1:12:A:LEU:H	1:12:A:LEU:HD21	2	0.1	0.0	0.1
(2,272)	1:12:A:LEU:H	1:12:A:LEU:HD22	2	0.1	0.0	0.1
(2,272)	1:12:A:LEU:H	1:12:A:LEU:HD23	2	0.1	0.0	0.1
(3,246)	1:12:A:LEU:H	1:12:A:LEU:HD21	2	0.1	0.0	0.1
(3,246)	1:12:A:LEU:H	1:12:A:LEU:HD22	2	0.1	0.0	0.1
(3,246)	1:12:A:LEU:H	1:12:A:LEU:HD23	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:1:A:GLU:HA	1:1:A:GLU:HB2	9	3.88
(1,669)	1:1:A:GLU:HA	1:1:A:GLU:HB2	7	3.82
(1,669)	1:1:A:GLU:HA	1:1:A:GLU:HB2	1	3.8
(1,669)	1:1:A:GLU:HA	1:1:A:GLU:HB2	2	3.28
(1,669)	1:1:A:GLU:HA	1:1:A:GLU:HB2	3	3.28
(1,669)	1:1:A:GLU:HA	1:1:A:GLU:HB2	5	3.28
(1,669)	1:1:A:GLU:HA	1:1:A:GLU:HB2	6	3.28
(1,669)	1:1:A:GLU:HA	1:1:A:GLU:HB2	8	3.28
(1,669)	1:1:A:GLU:HA	1:1:A:GLU:HB2	10	3.28
(1,669)	1:1:A:GLU:HA	1:1:A:GLU:HB2	4	3.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	3	3.03
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	3	3.03
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	3	3.03
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	3	3.03
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	3	3.03
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	3	3.03
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	3	3.03
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	3	3.03
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	3	3.03
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	3	3.03
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	3	3.03
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	3	3.03
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	3	3.03
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	3	3.03
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	3	3.03
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	3	3.03
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	3	3.03
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	3	3.03
(3,588)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	10	2.98
(2,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	10	2.98
(3,588)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	1	2.97
(2,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	1	2.97
(3,588)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	9	2.93
(2,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	9	2.93
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	1	2.91
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	1	2.91
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	1	2.91
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	1	2.91
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	1	2.91
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	1	2.91
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	1	2.91
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	1	2.91
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	1	2.91
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	1	2.91
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	1	2.91
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	1	2.91
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	1	2.91
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	1	2.91
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	1	2.91
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	1	2.91
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	1	2.91
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	1	2.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	4	2.9
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	4	2.9
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	4	2.9
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	4	2.9
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	4	2.9
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	4	2.9
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	4	2.9
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	4	2.9
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	4	2.9
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	10	2.9
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	10	2.9
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	10	2.9
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	10	2.9
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	10	2.9
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	10	2.9
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	10	2.9
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	10	2.9
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	10	2.9
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	4	2.9
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	4	2.9
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	4	2.9
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	4	2.9
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	4	2.9
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	4	2.9
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	4	2.9
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	4	2.9
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	4	2.9
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	10	2.9
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	10	2.9
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	10	2.9
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	10	2.9
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	10	2.9
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	10	2.9
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	10	2.9
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	10	2.9
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	10	2.9
(4,42)	1:6:A:ARG:H	1:9:A:ILE:HG12	2	2.88
(2,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	2	2.88
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	6	2.84
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	6	2.84
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	6	2.84
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	6	2.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	6	2.84
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	6	2.84
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	6	2.84
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	6	2.84
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	6	2.84
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	6	2.84
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	6	2.84
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	6	2.84
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	6	2.84
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	6	2.84
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	6	2.84
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	6	2.84
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	6	2.84
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	6	2.84
(4,42)	1:6:A:ARG:H	1:9:A:ILE:HG12	7	2.82
(2,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	7	2.82
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	9	2.78
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	9	2.78
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	9	2.78
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	9	2.78
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	9	2.78
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	9	2.78
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	9	2.78
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	9	2.78
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	9	2.78
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	9	2.78
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	9	2.78
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	9	2.78
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	9	2.78
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	9	2.78
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	9	2.78
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	9	2.78
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	9	2.78
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	9	2.78
(4,42)	1:6:A:ARG:H	1:9:A:ILE:HG12	5	2.76
(2,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	5	2.76
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	8	2.75
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	8	2.75
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	8	2.75
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	8	2.75
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	8	2.75
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	8	2.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	8	2.75
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	8	2.75
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	8	2.75
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	8	2.75
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	8	2.75
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	8	2.75
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	8	2.75
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	8	2.75
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	8	2.75
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	8	2.75
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	8	2.75
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	8	2.75
(4,35)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	3	2.7
(2,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	3	2.7
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	5	2.65
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	5	2.65
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	5	2.65
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	5	2.65
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	5	2.65
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	5	2.65
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	5	2.65
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	5	2.65
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	5	2.65
(4,35)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	2	2.65
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	5	2.65
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	5	2.65
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	5	2.65
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	5	2.65
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	5	2.65
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	5	2.65
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	5	2.65
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	5	2.65
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	5	2.65
(2,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	2	2.65
(3,588)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	6	2.63
(2,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	6	2.63
(4,35)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	7	2.62
(2,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	7	2.62
(4,35)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	6	2.61
(2,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	6	2.61
(4,35)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	2.6
(2,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	2.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	5	2.54
(2,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	5	2.54
(4,35)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	4	2.53
(4,35)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	9	2.53
(2,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	4	2.53
(2,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	9	2.53
(4,35)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	1	2.52
(2,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	1	2.52
(4,35)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	8	2.5
(2,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	8	2.5
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	3	2.38
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	3	2.38
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	3	2.38
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	3	2.38
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	3	2.38
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	3	2.38
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	3	2.38
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	3	2.38
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	3	2.38
(1,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	10	2.33
(1,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	1	2.32
(3,594)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	2	2.31
(3,594)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	2	2.31
(3,594)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	2	2.31
(2,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	2	2.31
(2,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	2	2.31
(2,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	2	2.31
(1,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	9	2.28
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	1	2.26
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	1	2.26
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	1	2.26
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	1	2.26
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	1	2.26
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	1	2.26
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	1	2.26
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	1	2.26
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	1	2.26
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	4	2.25
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	4	2.25
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	4	2.25
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	4	2.25
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	4	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	4	2.25
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	4	2.25
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	4	2.25
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	4	2.25
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	10	2.25
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	10	2.25
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	10	2.25
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	10	2.25
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	10	2.25
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	10	2.25
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	10	2.25
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	10	2.25
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	10	2.25
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	2	2.22
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	2	2.22
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	2	2.22
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	2	2.22
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	2	2.22
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	2	2.22
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	2	2.22
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	2	2.22
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	2	2.22
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	2	2.22
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	2	2.22
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	2	2.22
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	2	2.22
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	2	2.22
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	2	2.22
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	2	2.22
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	2	2.22
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	2	2.22
(1,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	2	2.22
(3,594)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	7	2.21
(3,594)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	7	2.21
(3,594)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	7	2.21
(2,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	7	2.21
(2,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	7	2.21
(2,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	7	2.21
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	2	2.2
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	2	2.2
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	2	2.2
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	7	2.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	7	2.2
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	7	2.2
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	6	2.19
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	6	2.19
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	6	2.19
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	6	2.19
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	6	2.19
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	6	2.19
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	6	2.19
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	6	2.19
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	6	2.19
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	7	2.18
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	7	2.18
(4,46)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	7	2.18
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	7	2.18
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	7	2.18
(4,46)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	7	2.18
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	7	2.18
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	7	2.18
(4,46)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	7	2.18
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	7	2.18
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	7	2.18
(2,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	7	2.18
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	7	2.18
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	7	2.18
(2,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	7	2.18
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	7	2.18
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	7	2.18
(2,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	7	2.18
(1,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	7	2.17
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	9	2.13
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	9	2.13
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	9	2.13
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	9	2.13
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	9	2.13
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	9	2.13
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	9	2.13
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	9	2.13
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	9	2.13
(1,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	5	2.11
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	8	2.09
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	8	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	8	2.09
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	8	2.09
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	8	2.09
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	8	2.09
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	8	2.09
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	8	2.09
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	8	2.09
(1,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	3	2.09
(1,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	2	2.04
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	2	2.02
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	2	2.02
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	2	2.02
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	2	2.02
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	2	2.02
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	2	2.02
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	2	2.02
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	2	2.02
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	2	2.02
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	2	2.02
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	2	2.02
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	2	2.02
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	2	2.02
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	2	2.02
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	2	2.02
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	2	2.02
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	2	2.02
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	2	2.02
(1,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	6	2.01
(1,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	7	2.01
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	5	2.0
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	5	2.0
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	5	2.0
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	5	2.0
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	5	2.0
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	5	2.0
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	5	2.0
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	5	2.0
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	5	2.0
(1,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	2.0
(4,8)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.99
(2,101)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.99
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	7	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	7	1.98
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	7	1.98
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	7	1.98
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	7	1.98
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	7	1.98
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	7	1.98
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	7	1.98
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	7	1.98
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	7	1.98
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	7	1.98
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	7	1.98
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	7	1.98
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	7	1.98
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	7	1.98
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	7	1.98
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	7	1.98
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	7	1.98
(1,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	6	1.97
(1,106)	1:6:A:ARG:HG3	1:7:A:LEU:H	7	1.97
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	7	1.93
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	7	1.93
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	7	1.93
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	7	1.93
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	7	1.93
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	7	1.93
(1,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	4	1.93
(1,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	5	1.93
(1,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	9	1.93
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	2	1.92
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	2	1.92
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	2	1.92
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	2	1.92
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	2	1.92
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	2	1.92
(1,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	1	1.92
(1,474)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	8	1.9
(4,42)	1:6:A:ARG:H	1:9:A:ILE:HG12	9	1.89
(2,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	9	1.89
(4,8)	1:9:A:ILE:HB	1:11:A:TRP:H	8	1.88
(2,101)	1:9:A:ILE:HB	1:11:A:TRP:H	8	1.88
(4,42)	1:6:A:ARG:H	1:9:A:ILE:HG12	1	1.87
(2,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	1	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,42)	1:6:A:ARG:H	1:9:A:ILE:HG12	6	1.86
(4,42)	1:6:A:ARG:H	1:9:A:ILE:HG12	8	1.86
(2,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	6	1.86
(2,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	8	1.86
(4,42)	1:6:A:ARG:H	1:9:A:ILE:HG12	10	1.85
(2,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	10	1.85
(4,42)	1:6:A:ARG:H	1:9:A:ILE:HG12	3	1.84
(4,24)	1:8:A:TYR:HD1	1:12:A:LEU:HG	1	1.84
(4,24)	1:8:A:TYR:HD2	1:12:A:LEU:HG	1	1.84
(4,24)	1:8:A:TYR:HD1	1:12:A:LEU:HG	6	1.84
(4,24)	1:8:A:TYR:HD2	1:12:A:LEU:HG	6	1.84
(3,587)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	6	1.84
(2,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	6	1.84
(2,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	3	1.84
(2,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	1	1.84
(2,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	1	1.84
(2,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	6	1.84
(2,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	6	1.84
(4,42)	1:6:A:ARG:H	1:9:A:ILE:HG12	4	1.83
(4,24)	1:8:A:TYR:HD1	1:12:A:LEU:HG	3	1.83
(4,24)	1:8:A:TYR:HD2	1:12:A:LEU:HG	3	1.83
(4,8)	1:9:A:ILE:HB	1:11:A:TRP:H	5	1.83
(2,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	4	1.83
(2,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	3	1.83
(2,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	3	1.83
(2,101)	1:9:A:ILE:HB	1:11:A:TRP:H	5	1.83
(4,24)	1:8:A:TYR:HD1	1:12:A:LEU:HG	4	1.82
(4,24)	1:8:A:TYR:HD2	1:12:A:LEU:HG	4	1.82
(4,24)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	1.82
(4,24)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	1.82
(4,24)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	1.82
(4,24)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	1.82
(2,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	4	1.82
(2,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	4	1.82
(2,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	1.82
(2,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	1.82
(2,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	1.82
(2,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	1.82
(3,587)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	9	1.81
(2,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	9	1.81
(4,8)	1:9:A:ILE:HB	1:11:A:TRP:H	9	1.79
(2,101)	1:9:A:ILE:HB	1:11:A:TRP:H	9	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,587)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	10	1.78
(2,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	10	1.78
(3,587)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	1	1.77
(2,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	1	1.77
(4,24)	1:8:A:TYR:HD1	1:12:A:LEU:HG	9	1.75
(4,24)	1:8:A:TYR:HD2	1:12:A:LEU:HG	9	1.75
(2,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	9	1.75
(2,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	9	1.75
(1,578)	1:19:A:SER:H	1:20:A:GLY:H	2	1.74
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	8	1.74
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	8	1.74
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	8	1.74
(4,26)	1:8:A:TYR:H	1:9:A:ILE:HB	3	1.73
(4,8)	1:9:A:ILE:HB	1:11:A:TRP:H	1	1.73
(4,8)	1:9:A:ILE:HB	1:11:A:TRP:H	4	1.73
(4,8)	1:9:A:ILE:HB	1:11:A:TRP:H	7	1.73
(2,271)	1:8:A:TYR:H	1:9:A:ILE:HB	3	1.73
(2,101)	1:9:A:ILE:HB	1:11:A:TRP:H	1	1.73
(2,101)	1:9:A:ILE:HB	1:11:A:TRP:H	4	1.73
(2,101)	1:9:A:ILE:HB	1:11:A:TRP:H	7	1.73
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	9	1.73
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	9	1.73
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	9	1.73
(4,8)	1:9:A:ILE:HB	1:11:A:TRP:H	6	1.72
(2,101)	1:9:A:ILE:HB	1:11:A:TRP:H	6	1.72
(4,8)	1:9:A:ILE:HB	1:11:A:TRP:H	3	1.71
(2,101)	1:9:A:ILE:HB	1:11:A:TRP:H	3	1.71
(4,26)	1:8:A:TYR:H	1:9:A:ILE:HB	4	1.7
(4,26)	1:8:A:TYR:H	1:9:A:ILE:HB	8	1.7
(4,24)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	1.7
(4,24)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	1.7
(2,271)	1:8:A:TYR:H	1:9:A:ILE:HB	4	1.7
(2,271)	1:8:A:TYR:H	1:9:A:ILE:HB	8	1.7
(2,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	1.7
(2,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	1.7
(1,578)	1:19:A:SER:H	1:20:A:GLY:H	5	1.7
(1,578)	1:19:A:SER:H	1:20:A:GLY:H	6	1.7
(4,8)	1:9:A:ILE:HB	1:11:A:TRP:H	2	1.69
(2,101)	1:9:A:ILE:HB	1:11:A:TRP:H	2	1.69
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	2	1.69
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	2	1.69
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	2	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	10	1.68
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	10	1.68
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	10	1.68
(1,578)	1:19:A:SER:H	1:20:A:GLY:H	4	1.67
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	7	1.67
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	7	1.67
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	7	1.67
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	7	1.66
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	7	1.66
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	7	1.66
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	7	1.66
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	7	1.66
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	7	1.66
(1,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	2	1.66
(1,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	2	1.66
(1,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	2	1.66
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	6	1.66
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	6	1.66
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	6	1.66
(1,578)	1:19:A:SER:H	1:20:A:GLY:H	10	1.65
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	3	1.65
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	3	1.65
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	3	1.65
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	5	1.65
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	5	1.65
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	5	1.65
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	2	1.64
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	2	1.64
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	2	1.64
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	2	1.64
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	2	1.64
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	2	1.64
(1,578)	1:19:A:SER:H	1:20:A:GLY:H	3	1.64
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	4	1.64
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	4	1.64
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	4	1.64
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	5	1.63
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	5	1.63
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	5	1.63
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	1	1.63
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	1	1.63
(1,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	1	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,586)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	10	1.62
(2,631)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	10	1.62
(3,586)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	1	1.61
(2,631)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	1	1.61
(1,578)	1:19:A:SER:H	1:20:A:GLY:H	7	1.59
(1,578)	1:19:A:SER:H	1:20:A:GLY:H	9	1.59
(3,586)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	9	1.58
(2,631)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	9	1.58
(1,665)	1:10:A:GLN:HA	1:13:A:LYS:HD3	10	1.58
(4,38)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	2	1.57
(4,38)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	2	1.57
(4,38)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	2	1.57
(4,26)	1:8:A:TYR:H	1:9:A:ILE:HB	6	1.57
(2,525)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	2	1.57
(2,525)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	2	1.57
(2,525)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	2	1.57
(2,271)	1:8:A:TYR:H	1:9:A:ILE:HB	6	1.57
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	7	1.57
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	7	1.57
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	7	1.57
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	6	1.57
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	6	1.57
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	10	1.57
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	10	1.57
(4,26)	1:8:A:TYR:H	1:9:A:ILE:HB	9	1.56
(2,271)	1:8:A:TYR:H	1:9:A:ILE:HB	9	1.56
(1,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	7	1.56
(1,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	7	1.56
(1,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	7	1.56
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	2	1.56
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	2	1.56
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	2	1.56
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	2	1.56
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	2	1.56
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	2	1.56
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	2	1.56
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	2	1.56
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	2	1.56
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	1	1.56
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	1	1.56
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG2	1	1.55
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG3	1	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,258)	1:12:A:LEU:HD11	1:16:A:GLY:H	2	1.54
(3,258)	1:12:A:LEU:HD12	1:16:A:GLY:H	2	1.54
(3,258)	1:12:A:LEU:HD13	1:16:A:GLY:H	2	1.54
(2,287)	1:12:A:LEU:HD11	1:16:A:GLY:H	2	1.54
(2,287)	1:12:A:LEU:HD12	1:16:A:GLY:H	2	1.54
(2,287)	1:12:A:LEU:HD13	1:16:A:GLY:H	2	1.54
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG2	6	1.54
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG3	6	1.54
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD11	7	1.53
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD12	7	1.53
(1,639)	1:5:A:VAL:HG21	1:12:A:LEU:HD13	7	1.53
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD11	7	1.53
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD12	7	1.53
(1,639)	1:5:A:VAL:HG22	1:12:A:LEU:HD13	7	1.53
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD11	7	1.53
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD12	7	1.53
(1,639)	1:5:A:VAL:HG23	1:12:A:LEU:HD13	7	1.53
(4,15)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	1.52
(2,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	1.52
(1,532)	1:9:A:ILE:HA	1:12:A:LEU:HG	7	1.52
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG2	8	1.51
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG3	8	1.51
(1,665)	1:10:A:GLN:HA	1:13:A:LYS:HD3	6	1.51
(4,26)	1:8:A:TYR:H	1:9:A:ILE:HB	1	1.5
(4,15)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	1.5
(4,15)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	1.5
(4,15)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	1.5
(2,271)	1:8:A:TYR:H	1:9:A:ILE:HB	1	1.5
(2,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	1.5
(2,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	1.5
(2,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	1.5
(1,532)	1:9:A:ILE:HA	1:12:A:LEU:HG	2	1.5
(4,15)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	1.49
(4,15)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	1.49
(4,15)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.49
(2,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	1.49
(2,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	1.49
(2,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.49
(4,15)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	1.48
(4,15)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	1.48
(2,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	1.48
(2,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,26)	1:8:A:TYR:H	1:9:A:ILE:HB	10	1.47
(4,15)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	1.47
(3,258)	1:12:A:LEU:HD11	1:16:A:GLY:H	7	1.47
(3,258)	1:12:A:LEU:HD12	1:16:A:GLY:H	7	1.47
(3,258)	1:12:A:LEU:HD13	1:16:A:GLY:H	7	1.47
(2,287)	1:12:A:LEU:HD11	1:16:A:GLY:H	7	1.47
(2,287)	1:12:A:LEU:HD12	1:16:A:GLY:H	7	1.47
(2,287)	1:12:A:LEU:HD13	1:16:A:GLY:H	7	1.47
(2,271)	1:8:A:TYR:H	1:9:A:ILE:HB	10	1.47
(2,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	1.47
(4,38)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	7	1.46
(4,38)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	7	1.46
(4,38)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	7	1.46
(2,525)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	7	1.46
(2,525)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	7	1.46
(2,525)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	7	1.46
(1,601)	1:8:A:TYR:HD1	1:25:A:CYS:HB3	5	1.46
(1,601)	1:8:A:TYR:HD2	1:25:A:CYS:HB3	5	1.46
(4,30)	1:10:A:GLN:HE22	1:11:A:TRP:H	4	1.45
(2,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	4	1.45
(1,261)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	4	1.45
(1,261)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	2	1.43
(4,30)	1:10:A:GLN:HE22	1:11:A:TRP:H	5	1.42
(4,30)	1:10:A:GLN:HE22	1:11:A:TRP:H	7	1.42
(2,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	5	1.42
(2,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	7	1.42
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	2	1.42
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	2	1.42
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	2	1.42
(4,26)	1:8:A:TYR:H	1:9:A:ILE:HB	2	1.41
(2,271)	1:8:A:TYR:H	1:9:A:ILE:HB	2	1.41
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	3	1.41
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	3	1.41
(1,261)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	8	1.41
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	7	1.4
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	7	1.4
(1,122)	1:10:A:GLN:HA	1:10:A:GLN:HE21	10	1.4
(3,578)	1:5:A:VAL:HA	1:25:A:CYS:HB2	9	1.39
(2,623)	1:5:A:VAL:HA	1:25:A:CYS:HB2	9	1.39
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	2	1.39
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	2	1.39
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	5	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	5	1.39
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	8	1.39
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	8	1.39
(1,261)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	1	1.39
(1,665)	1:10:A:GLN:HA	1:13:A:LYS:HD3	3	1.38
(1,443)	1:22:A:PRO:HA	1:22:A:PRO:HD2	1	1.38
(1,443)	1:22:A:PRO:HA	1:22:A:PRO:HD2	2	1.38
(1,443)	1:22:A:PRO:HA	1:22:A:PRO:HD2	3	1.38
(1,261)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	5	1.38
(1,122)	1:10:A:GLN:HA	1:10:A:GLN:HE21	2	1.38
(4,26)	1:8:A:TYR:H	1:9:A:ILE:HB	5	1.36
(2,271)	1:8:A:TYR:H	1:9:A:ILE:HB	5	1.36
(1,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	2	1.36
(1,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	2	1.36
(1,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	2	1.36
(1,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	2	1.36
(1,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	2	1.36
(1,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	2	1.36
(1,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	2	1.36
(1,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	2	1.36
(1,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	2	1.36
(1,627)	1:14:A:ASP:HB3	1:19:A:SER:HB2	8	1.36
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	4	1.36
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	4	1.36
(3,586)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	6	1.35
(3,202)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	10	1.35
(3,144)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	5	1.35
(2,631)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	6	1.35
(2,227)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	10	1.35
(2,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	5	1.35
(1,647)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	3	1.35
(1,647)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	3	1.35
(1,647)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	3	1.35
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	9	1.35
(1,522)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	9	1.35
(4,30)	1:10:A:GLN:HE22	1:11:A:TRP:H	6	1.34
(3,202)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	7	1.34
(2,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	6	1.34
(2,227)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	7	1.34
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	3	1.34
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	3	1.34
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	3	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	3	1.34
(1,261)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	9	1.34
(1,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	7	1.34
(1,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	7	1.34
(1,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	7	1.34
(1,122)	1:10:A:GLN:HA	1:10:A:GLN:HE21	4	1.34
(3,144)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	4	1.33
(2,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	4	1.33
(1,635)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	2	1.33
(1,635)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	2	1.33
(1,635)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	2	1.33
(1,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	2	1.33
(1,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	2	1.33
(1,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	2	1.33
(1,101)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.33
(3,202)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	5	1.32
(3,202)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	8	1.32
(3,144)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	1	1.32
(3,144)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	7	1.32
(3,144)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	8	1.32
(3,144)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	1.32
(2,227)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	5	1.32
(2,227)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	8	1.32
(2,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	1	1.32
(2,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	7	1.32
(2,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	8	1.32
(2,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	1.32
(1,647)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	4	1.32
(1,647)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	4	1.32
(1,647)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	4	1.32
(1,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	7	1.32
(1,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	7	1.32
(1,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	7	1.32
(1,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	7	1.32
(1,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	7	1.32
(1,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	7	1.32
(1,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	7	1.32
(1,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	7	1.32
(1,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	7	1.32
(1,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	3	1.32
(1,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	3	1.32
(1,122)	1:10:A:GLN:HA	1:10:A:GLN:HE21	7	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,144)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	3	1.31
(3,144)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	6	1.31
(3,144)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	9	1.31
(2,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	3	1.31
(2,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	6	1.31
(2,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	9	1.31
(3,503)	1:4:A:CYS:HA	1:7:A:LEU:HB2	6	1.3
(3,202)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	9	1.3
(2,541)	1:4:A:CYS:HA	1:7:A:LEU:HB2	6	1.3
(2,227)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	9	1.3
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	5	1.3
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	5	1.3
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	5	1.3
(1,601)	1:8:A:TYR:HD1	1:25:A:CYS:HB3	2	1.3
(1,601)	1:8:A:TYR:HD2	1:25:A:CYS:HB3	2	1.3
(1,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	6	1.3
(1,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	6	1.3
(1,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	9	1.3
(1,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	9	1.3
(3,172)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	7	1.29
(2,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	7	1.29
(1,635)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	1	1.29
(1,635)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	1	1.29
(1,635)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	1	1.29
(1,567)	1:12:A:LEU:HA	1:16:A:GLY:HA2	8	1.29
(1,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	8	1.29
(1,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	8	1.29
(4,30)	1:10:A:GLN:HE22	1:11:A:TRP:H	9	1.28
(4,26)	1:8:A:TYR:H	1:9:A:ILE:HB	7	1.28
(3,202)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	3	1.28
(3,202)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	4	1.28
(3,172)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	2	1.28
(2,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	9	1.28
(2,271)	1:8:A:TYR:H	1:9:A:ILE:HB	7	1.28
(2,227)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	3	1.28
(2,227)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	4	1.28
(2,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	2	1.28
(1,647)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	6	1.28
(1,647)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	6	1.28
(1,647)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	6	1.28
(1,647)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	10	1.28
(1,647)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	10	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	10	1.28
(1,443)	1:22:A:PRO:HA	1:22:A:PRO:HD2	8	1.28
(1,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	1	1.28
(1,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	1	1.28
(1,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	4	1.28
(1,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	4	1.28
(1,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	10	1.28
(1,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	10	1.28
(1,443)	1:22:A:PRO:HA	1:22:A:PRO:HD2	5	1.27
(1,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	2	1.27
(1,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	2	1.27
(1,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	7	1.27
(1,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	7	1.27
(4,30)	1:10:A:GLN:HE22	1:11:A:TRP:H	8	1.26
(4,22)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	1	1.26
(3,202)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	6	1.26
(3,144)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	2	1.26
(3,103)	1:7:A:LEU:H	1:10:A:GLN:HB3	2	1.26
(2,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	8	1.26
(2,227)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	6	1.26
(2,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	1	1.26
(2,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	2	1.26
(2,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	2	1.26
(1,647)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	1	1.26
(1,647)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	1	1.26
(1,647)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	1	1.26
(1,443)	1:22:A:PRO:HA	1:22:A:PRO:HD2	7	1.26
(1,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	5	1.26
(1,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	5	1.26
(4,30)	1:10:A:GLN:HE22	1:11:A:TRP:H	2	1.25
(3,345)	1:12:A:LEU:HA	1:12:A:LEU:HD11	2	1.25
(3,345)	1:12:A:LEU:HA	1:12:A:LEU:HD12	2	1.25
(3,345)	1:12:A:LEU:HA	1:12:A:LEU:HD13	2	1.25
(3,202)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	1	1.25
(2,377)	1:12:A:LEU:HA	1:12:A:LEU:HD11	2	1.25
(2,377)	1:12:A:LEU:HA	1:12:A:LEU:HD12	2	1.25
(2,377)	1:12:A:LEU:HA	1:12:A:LEU:HD13	2	1.25
(2,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	2	1.25
(2,227)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	1	1.25
(1,443)	1:22:A:PRO:HA	1:22:A:PRO:HD2	4	1.25
(3,578)	1:5:A:VAL:HA	1:25:A:CYS:HB2	7	1.24
(3,345)	1:12:A:LEU:HA	1:12:A:LEU:HD11	7	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,345)	1:12:A:LEU:HA	1:12:A:LEU:HD12	7	1.24
(3,345)	1:12:A:LEU:HA	1:12:A:LEU:HD13	7	1.24
(3,173)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	7	1.24
(3,173)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	7	1.24
(3,173)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	7	1.24
(2,623)	1:5:A:VAL:HA	1:25:A:CYS:HB2	7	1.24
(2,377)	1:12:A:LEU:HA	1:12:A:LEU:HD11	7	1.24
(2,377)	1:12:A:LEU:HA	1:12:A:LEU:HD12	7	1.24
(2,377)	1:12:A:LEU:HA	1:12:A:LEU:HD13	7	1.24
(2,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	7	1.24
(2,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	7	1.24
(2,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	7	1.24
(1,647)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	8	1.24
(1,647)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	8	1.24
(1,647)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	8	1.24
(1,443)	1:22:A:PRO:HA	1:22:A:PRO:HD2	6	1.24
(1,443)	1:22:A:PRO:HA	1:22:A:PRO:HD2	9	1.24
(1,122)	1:10:A:GLN:HA	1:10:A:GLN:HE21	6	1.24
(1,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	9	1.23
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	2	1.23
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	2	1.23
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	2	1.23
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	2	1.23
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	3	1.23
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	3	1.23
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	3	1.23
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	3	1.23
(1,443)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	1.23
(1,122)	1:10:A:GLN:HA	1:10:A:GLN:HE21	5	1.23
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	2	1.22
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	2	1.22
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	2	1.22
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	2	1.22
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	2	1.22
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	2	1.22
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	7	1.22
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	7	1.22
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	7	1.22
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	7	1.22
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	7	1.22
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	7	1.22
(3,588)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	8	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	8	1.22
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	2	1.22
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	2	1.22
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	2	1.22
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	2	1.22
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	2	1.22
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	2	1.22
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	7	1.22
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	7	1.22
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	7	1.22
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	7	1.22
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	7	1.22
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	7	1.22
(1,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	1	1.22
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	5	1.22
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	5	1.22
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	5	1.22
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	5	1.22
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	8	1.22
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	8	1.22
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	8	1.22
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	8	1.22
(1,101)	1:9:A:ILE:HB	1:11:A:TRP:H	8	1.22
(3,172)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	8	1.21
(2,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	8	1.21
(1,665)	1:10:A:GLN:HA	1:13:A:LYS:HD3	9	1.21
(1,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	6	1.21
(1,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	8	1.21
(1,658)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	4	1.2
(1,658)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	4	1.2
(1,658)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	4	1.2
(1,647)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	9	1.2
(1,647)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	9	1.2
(1,647)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	9	1.2
(1,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	10	1.2
(4,36)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	9	1.19
(4,36)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	1.19
(4,30)	1:10:A:GLN:HE22	1:11:A:TRP:H	3	1.19
(3,173)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	2	1.19
(3,173)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	2	1.19
(3,173)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	2	1.19
(2,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	9	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	1.19
(2,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	3	1.19
(2,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	2	1.19
(2,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	2	1.19
(2,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	2	1.19
(1,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	3	1.19
(1,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	6	1.19
(1,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	6	1.19
(1,198)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	2	1.19
(1,198)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	2	1.19
(1,198)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	2	1.19
(4,36)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	1	1.18
(4,36)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	3	1.18
(4,36)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	6	1.18
(4,36)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	8	1.18
(3,202)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	2	1.18
(3,148)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	2	1.18
(2,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	1	1.18
(2,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	3	1.18
(2,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	6	1.18
(2,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	8	1.18
(2,227)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	2	1.18
(2,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	2	1.18
(1,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	6	1.18
(1,625)	1:8:A:TYR:HB2	1:25:A:CYS:HB3	9	1.18
(1,625)	1:8:A:TYR:HB3	1:25:A:CYS:HB3	9	1.18
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	6	1.18
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	6	1.18
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	6	1.18
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	6	1.18
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	6	1.18
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	6	1.18
(1,601)	1:8:A:TYR:HD1	1:25:A:CYS:HB3	8	1.18
(1,601)	1:8:A:TYR:HD2	1:25:A:CYS:HB3	8	1.18
(1,594)	1:6:A:ARG:H	1:9:A:ILE:HG12	4	1.18
(1,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	1	1.18
(1,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	1	1.18
(4,36)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	7	1.17
(2,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	7	1.17
(1,376)	1:12:A:LEU:HA	1:12:A:LEU:HD21	7	1.17
(1,376)	1:12:A:LEU:HA	1:12:A:LEU:HD22	7	1.17
(1,376)	1:12:A:LEU:HA	1:12:A:LEU:HD23	7	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	3	1.17
(1,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	3	1.17
(1,101)	1:9:A:ILE:HB	1:11:A:TRP:H	5	1.17
(4,36)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	4	1.16
(4,36)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	5	1.16
(4,22)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	2	1.16
(2,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	4	1.16
(2,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	5	1.16
(2,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	2	1.16
(1,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	9	1.16
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	4	1.16
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	4	1.16
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	4	1.16
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	4	1.16
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	4	1.16
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	4	1.16
(1,376)	1:12:A:LEU:HA	1:12:A:LEU:HD21	2	1.16
(1,376)	1:12:A:LEU:HA	1:12:A:LEU:HD22	2	1.16
(1,376)	1:12:A:LEU:HA	1:12:A:LEU:HD23	2	1.16
(1,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	4	1.16
(1,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	4	1.16
(1,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	1.16
(1,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	1.16
(1,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	1.16
(1,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	1.16
(1,625)	1:8:A:TYR:HB2	1:25:A:CYS:HB3	7	1.15
(1,625)	1:8:A:TYR:HB3	1:25:A:CYS:HB3	7	1.15
(1,610)	1:15:A:GLY:HA3	1:19:A:SER:HB3	3	1.15
(1,122)	1:10:A:GLN:HA	1:10:A:GLN:HE21	9	1.15
(4,9)	1:12:A:LEU:H	1:12:A:LEU:HG	5	1.14
(3,588)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	3	1.14
(2,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	3	1.14
(2,110)	1:12:A:LEU:H	1:12:A:LEU:HG	5	1.14
(1,610)	1:15:A:GLY:HA3	1:19:A:SER:HB3	1	1.14
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	3	1.14
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	3	1.14
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	3	1.14
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	3	1.14
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	3	1.14
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	3	1.14
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	10	1.14
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	10	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	10	1.14
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	10	1.14
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	10	1.14
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	10	1.14
(3,148)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	7	1.13
(2,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	7	1.13
(1,610)	1:15:A:GLY:HA3	1:19:A:SER:HB3	5	1.13
(1,101)	1:9:A:ILE:HB	1:11:A:TRP:H	9	1.13
(4,47)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	5	1.12
(4,47)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	5	1.12
(4,47)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	5	1.12
(4,36)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	2	1.12
(2,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	5	1.12
(2,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	5	1.12
(2,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	5	1.12
(2,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	2	1.12
(1,665)	1:10:A:GLN:HA	1:13:A:LYS:HD3	8	1.12
(1,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	10	1.12
(1,567)	1:12:A:LEU:HA	1:16:A:GLY:HA2	9	1.12
(1,198)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	7	1.12
(1,198)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	7	1.12
(1,198)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	7	1.12
(4,47)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	4	1.11
(4,47)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	4	1.11
(4,47)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	4	1.11
(2,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	4	1.11
(2,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	4	1.11
(2,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	4	1.11
(1,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	1	1.11
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	9	1.11
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	9	1.11
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	9	1.11
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	9	1.11
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	9	1.11
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	9	1.11
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG2	10	1.11
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG3	10	1.11
(1,610)	1:15:A:GLY:HA3	1:19:A:SER:HB3	6	1.1
(1,610)	1:15:A:GLY:HA3	1:19:A:SER:HB3	7	1.1
(3,588)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	4	1.09
(3,172)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	10	1.09
(2,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	4	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	10	1.09
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	8	1.09
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	8	1.09
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	8	1.09
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	8	1.09
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	8	1.09
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	8	1.09
(1,324)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	4	1.09
(1,324)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	6	1.09
(1,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	9	1.09
(1,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	9	1.09
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG2	7	1.09
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG3	7	1.09
(3,172)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	6	1.08
(2,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	6	1.08
(1,610)	1:15:A:GLY:HA3	1:19:A:SER:HB3	2	1.08
(1,610)	1:15:A:GLY:HA3	1:19:A:SER:HB3	10	1.08
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	4	1.08
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	4	1.08
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	4	1.08
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	4	1.08
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	9	1.08
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	9	1.08
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	9	1.08
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	9	1.08
(1,271)	1:8:A:TYR:H	1:9:A:ILE:HB	3	1.08
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG2	5	1.08
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG3	5	1.08
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG2	6	1.08
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG3	6	1.08
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG2	9	1.08
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG3	9	1.08
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	9	1.08
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	9	1.08
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	9	1.08
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	1	1.07
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	1	1.07
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	1	1.07
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	1	1.07
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	1	1.07
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	1	1.07
(1,101)	1:9:A:ILE:HB	1:11:A:TRP:H	1	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,101)	1:9:A:ILE:HB	1:11:A:TRP:H	4	1.07
(1,101)	1:9:A:ILE:HB	1:11:A:TRP:H	6	1.07
(1,101)	1:9:A:ILE:HB	1:11:A:TRP:H	7	1.07
(4,9)	1:12:A:LEU:H	1:12:A:LEU:HG	1	1.06
(4,9)	1:12:A:LEU:H	1:12:A:LEU:HG	6	1.06
(2,110)	1:12:A:LEU:H	1:12:A:LEU:HG	1	1.06
(2,110)	1:12:A:LEU:H	1:12:A:LEU:HG	6	1.06
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	2	1.06
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	2	1.06
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	2	1.06
(1,635)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	4	1.06
(1,635)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	4	1.06
(1,635)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	4	1.06
(1,627)	1:14:A:ASP:HB3	1:19:A:SER:HB2	9	1.06
(1,610)	1:15:A:GLY:HA3	1:19:A:SER:HB3	4	1.06
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG2	4	1.06
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG3	4	1.06
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	8	1.06
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	8	1.06
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	8	1.06
(4,30)	1:10:A:GLN:HE22	1:11:A:TRP:H	1	1.05
(4,9)	1:12:A:LEU:H	1:12:A:LEU:HG	3	1.05
(3,147)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	1.05
(2,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	1	1.05
(2,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	1.05
(2,110)	1:12:A:LEU:H	1:12:A:LEU:HG	3	1.05
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG2	5	1.05
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG3	5	1.05
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	8	1.05
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	8	1.05
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	8	1.05
(1,314)	1:6:A:ARG:HA	1:6:A:ARG:HD3	8	1.05
(1,271)	1:8:A:TYR:H	1:9:A:ILE:HB	4	1.05
(1,271)	1:8:A:TYR:H	1:9:A:ILE:HB	8	1.05
(1,122)	1:10:A:GLN:HA	1:10:A:GLN:HE21	8	1.05
(1,101)	1:9:A:ILE:HB	1:11:A:TRP:H	3	1.05
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG2	3	1.05
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG3	3	1.05
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG2	8	1.05
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG3	8	1.05
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	10	1.05
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	10	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	10	1.05
(4,9)	1:12:A:LEU:H	1:12:A:LEU:HG	4	1.04
(3,588)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	7	1.04
(3,172)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	9	1.04
(3,103)	1:7:A:LEU:H	1:10:A:GLN:HB3	4	1.04
(2,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	7	1.04
(2,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	9	1.04
(2,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	4	1.04
(2,110)	1:12:A:LEU:H	1:12:A:LEU:HG	4	1.04
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	9	1.04
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	9	1.04
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	9	1.04
(1,610)	1:15:A:GLY:HA3	1:19:A:SER:HB3	9	1.04
(1,567)	1:12:A:LEU:HA	1:16:A:GLY:HA2	7	1.04
(1,214)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	1.04
(1,214)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	1.04
(4,21)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	1	1.03
(4,21)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	1	1.03
(4,9)	1:12:A:LEU:H	1:12:A:LEU:HG	10	1.03
(3,509)	1:14:A:ASP:HB2	1:19:A:SER:HB3	5	1.03
(3,172)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	1	1.03
(3,147)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	1.03
(3,147)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	1.03
(3,147)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.03
(2,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	5	1.03
(2,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	1	1.03
(2,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	1	1.03
(2,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	1	1.03
(2,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	1.03
(2,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	1.03
(2,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.03
(2,110)	1:12:A:LEU:H	1:12:A:LEU:HG	10	1.03
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	5	1.03
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	5	1.03
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	5	1.03
(1,324)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	9	1.03
(1,314)	1:6:A:ARG:HA	1:6:A:ARG:HD3	1	1.03
(1,281)	1:24:A:PRO:HG2	1:25:A:CYS:H	1	1.03
(1,101)	1:9:A:ILE:HB	1:11:A:TRP:H	2	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	1	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	1	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	3	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	3	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	3	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	4	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	4	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	4	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	6	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	6	1.03
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	6	1.03
(4,47)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	1	1.02
(4,47)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	1	1.02
(4,47)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	1	1.02
(4,47)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	3	1.02
(4,47)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	3	1.02
(4,47)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	3	1.02
(3,550)	1:2:A:GLU:HB2	1:5:A:VAL:H	8	1.02
(3,147)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	1.02
(3,147)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	1.02
(3,147)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	1.02
(2,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	1	1.02
(2,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	1	1.02
(2,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	1	1.02
(2,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	3	1.02
(2,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	3	1.02
(2,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	3	1.02
(2,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	8	1.02
(2,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	1.02
(2,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	1.02
(2,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	1.02
(1,567)	1:12:A:LEU:HA	1:16:A:GLY:HA2	1	1.02
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	1	1.02
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	1	1.02
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	1	1.02
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	1	1.02
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	7	1.02
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	7	1.02
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	7	1.02
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	7	1.02
(1,281)	1:24:A:PRO:HG2	1:25:A:CYS:H	3	1.02
(4,6)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	1.01
(3,503)	1:4:A:CYS:HA	1:7:A:LEU:HB2	9	1.01
(2,541)	1:4:A:CYS:HA	1:7:A:LEU:HB2	9	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	1.01
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG2	3	1.01
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG3	3	1.01
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	7	1.01
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	7	1.01
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	7	1.01
(1,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	7	1.01
(1,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	7	1.01
(1,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	7	1.01
(1,625)	1:8:A:TYR:HB2	1:25:A:CYS:HB3	5	1.01
(1,625)	1:8:A:TYR:HB3	1:25:A:CYS:HB3	5	1.01
(3,147)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	1.0
(3,147)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	1.0
(2,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	1.0
(2,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	1.0
(1,625)	1:8:A:TYR:HB2	1:25:A:CYS:HB3	4	1.0
(1,625)	1:8:A:TYR:HB3	1:25:A:CYS:HB3	4	1.0
(1,559)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	2	1.0
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD11	9	1.0
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD12	9	1.0
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD13	9	1.0
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD21	9	1.0
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD22	9	1.0
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD23	9	1.0
(3,481)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	4	0.99
(3,481)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	4	0.99
(3,481)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	4	0.99
(3,147)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	0.99
(3,8)	1:9:A:ILE:H	1:12:A:LEU:HD21	2	0.99
(3,8)	1:9:A:ILE:H	1:12:A:LEU:HD22	2	0.99
(3,8)	1:9:A:ILE:H	1:12:A:LEU:HD23	2	0.99
(2,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	4	0.99
(2,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	4	0.99
(2,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	4	0.99
(2,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	0.99
(2,10)	1:9:A:ILE:H	1:12:A:LEU:HD21	2	0.99
(2,10)	1:9:A:ILE:H	1:12:A:LEU:HD22	2	0.99
(2,10)	1:9:A:ILE:H	1:12:A:LEU:HD23	2	0.99
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	9	0.99
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	9	0.99
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	9	0.99
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	5	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	5	0.99
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	5	0.99
(1,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	2	0.99
(1,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	2	0.99
(1,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	2	0.99
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	6	0.99
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	6	0.99
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	6	0.99
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	6	0.99
(1,287)	1:12:A:LEU:HD11	1:16:A:GLY:H	2	0.99
(1,287)	1:12:A:LEU:HD12	1:16:A:GLY:H	2	0.99
(1,287)	1:12:A:LEU:HD13	1:16:A:GLY:H	2	0.99
(1,281)	1:24:A:PRO:HG2	1:25:A:CYS:H	10	0.99
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG2	1	0.99
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG3	1	0.99
(3,575)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	4	0.98
(3,503)	1:4:A:CYS:HA	1:7:A:LEU:HB2	10	0.98
(3,461)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	2	0.98
(2,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	4	0.98
(2,541)	1:4:A:CYS:HA	1:7:A:LEU:HB2	10	0.98
(2,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	2	0.98
(1,577)	1:20:A:GLY:H	1:21:A:ARG:H	1	0.98
(1,559)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	4	0.98
(1,559)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	6	0.98
(1,472)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	2	0.98
(1,244)	1:8:A:TYR:HD1	1:9:A:ILE:H	3	0.98
(1,244)	1:8:A:TYR:HD2	1:9:A:ILE:H	3	0.98
(1,244)	1:8:A:TYR:HD1	1:9:A:ILE:H	10	0.98
(1,244)	1:8:A:TYR:HD2	1:9:A:ILE:H	10	0.98
(1,212)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	1	0.98
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG2	2	0.98
(1,53)	1:21:A:ARG:H	1:21:A:ARG:HG3	2	0.98
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	5	0.97
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	5	0.97
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	5	0.97
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	5	0.97
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	5	0.97
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	5	0.97
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	5	0.97
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	5	0.97
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	5	0.97
(4,21)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	4	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,21)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	4	0.97
(3,575)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	5	0.97
(3,575)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	10	0.97
(3,172)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	3	0.97
(3,103)	1:7:A:LEU:H	1:10:A:GLN:HB3	9	0.97
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	5	0.97
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	5	0.97
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	5	0.97
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	5	0.97
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	5	0.97
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	5	0.97
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	5	0.97
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	5	0.97
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	5	0.97
(2,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	5	0.97
(2,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	10	0.97
(2,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	4	0.97
(2,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	4	0.97
(2,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	3	0.97
(2,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	9	0.97
(1,631)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	10	0.97
(1,630)	1:2:A:GLU:HG2	1:5:A:VAL:HB	9	0.97
(1,630)	1:2:A:GLU:HG3	1:5:A:VAL:HB	9	0.97
(1,577)	1:20:A:GLY:H	1:21:A:ARG:H	8	0.97
(1,567)	1:12:A:LEU:HA	1:16:A:GLY:HA2	2	0.97
(1,567)	1:12:A:LEU:HA	1:16:A:GLY:HA2	10	0.97
(1,559)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	9	0.97
(1,314)	1:6:A:ARG:HA	1:6:A:ARG:HD3	10	0.97
(1,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	0.97
(1,122)	1:10:A:GLN:HA	1:10:A:GLN:HE21	3	0.97
(4,47)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	6	0.96
(4,47)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	6	0.96
(4,47)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	6	0.96
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	8	0.96
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	8	0.96
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	8	0.96
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	8	0.96
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	8	0.96
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	8	0.96
(3,503)	1:4:A:CYS:HA	1:7:A:LEU:HB2	1	0.96
(3,103)	1:7:A:LEU:H	1:10:A:GLN:HB3	5	0.96
(3,8)	1:9:A:ILE:H	1:12:A:LEU:HD21	7	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,8)	1:9:A:ILE:H	1:12:A:LEU:HD22	7	0.96
(3,8)	1:9:A:ILE:H	1:12:A:LEU:HD23	7	0.96
(2,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	6	0.96
(2,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	6	0.96
(2,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	6	0.96
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	8	0.96
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	8	0.96
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	8	0.96
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	8	0.96
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	8	0.96
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	8	0.96
(2,541)	1:4:A:CYS:HA	1:7:A:LEU:HB2	1	0.96
(2,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	5	0.96
(2,10)	1:9:A:ILE:H	1:12:A:LEU:HD21	7	0.96
(2,10)	1:9:A:ILE:H	1:12:A:LEU:HD22	7	0.96
(2,10)	1:9:A:ILE:H	1:12:A:LEU:HD23	7	0.96
(1,631)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	1	0.96
(1,625)	1:8:A:TYR:HB2	1:25:A:CYS:HB3	8	0.96
(1,625)	1:8:A:TYR:HB3	1:25:A:CYS:HB3	8	0.96
(1,567)	1:12:A:LEU:HA	1:16:A:GLY:HA2	6	0.96
(1,559)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	3	0.96
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD11	1	0.96
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD12	1	0.96
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD13	1	0.96
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD21	1	0.96
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD22	1	0.96
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD23	1	0.96
(1,324)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	7	0.96
(1,314)	1:6:A:ARG:HA	1:6:A:ARG:HD3	5	0.96
(4,47)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	10	0.95
(4,47)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	10	0.95
(4,47)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	10	0.95
(3,575)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	6	0.95
(3,575)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	7	0.95
(3,575)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	9	0.95
(3,172)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	5	0.95
(2,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	10	0.95
(2,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	10	0.95
(2,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	10	0.95
(2,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	6	0.95
(2,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	7	0.95
(2,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	9	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	5	0.95
(1,630)	1:2:A:GLU:HG2	1:5:A:VAL:HB	1	0.95
(1,630)	1:2:A:GLU:HG3	1:5:A:VAL:HB	1	0.95
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	3	0.95
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	3	0.95
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	3	0.95
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	3	0.95
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	3	0.95
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	3	0.95
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	10	0.95
(1,523)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	10	0.95
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	10	0.95
(1,523)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	10	0.95
(1,281)	1:24:A:PRO:HG2	1:25:A:CYS:H	6	0.95
(1,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	0.95
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	3	0.94
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	3	0.94
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	3	0.94
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	3	0.94
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	3	0.94
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	3	0.94
(4,9)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.94
(3,575)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	8	0.94
(3,567)	1:15:A:GLY:HA3	1:18:A:SER:HB3	6	0.94
(3,509)	1:14:A:ASP:HB2	1:19:A:SER:HB3	2	0.94
(3,509)	1:14:A:ASP:HB2	1:19:A:SER:HB3	3	0.94
(3,461)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	4	0.94
(3,172)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	4	0.94
(3,145)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	6	0.94
(2,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	8	0.94
(2,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	6	0.94
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	3	0.94
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	3	0.94
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	3	0.94
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	3	0.94
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	3	0.94
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	3	0.94
(2,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	2	0.94
(2,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	3	0.94
(2,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	4	0.94
(2,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	4	0.94
(2,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	6	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.94
(1,635)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	9	0.94
(1,635)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	9	0.94
(1,635)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	9	0.94
(1,628)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	9	0.94
(1,601)	1:8:A:TYR:HD1	1:25:A:CYS:HB3	4	0.94
(1,601)	1:8:A:TYR:HD2	1:25:A:CYS:HB3	4	0.94
(1,588)	1:14:A:ASP:HB3	1:15:A:GLY:H	7	0.94
(1,577)	1:20:A:GLY:H	1:21:A:ARG:H	2	0.94
(1,577)	1:20:A:GLY:H	1:21:A:ARG:H	4	0.94
(1,525)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	2	0.94
(1,525)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	2	0.94
(1,525)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	2	0.94
(1,244)	1:8:A:TYR:HD1	1:9:A:ILE:H	6	0.94
(1,244)	1:8:A:TYR:HD2	1:9:A:ILE:H	6	0.94
(1,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	0.94
(1,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	0.94
(1,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	0.94
(1,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	0.94
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	4	0.93
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	4	0.93
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	4	0.93
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	4	0.93
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	4	0.93
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	4	0.93
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	9	0.93
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	9	0.93
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	9	0.93
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	9	0.93
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	9	0.93
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	9	0.93
(4,23)	1:11:A:TRP:HE3	1:12:A:LEU:HG	5	0.93
(3,611)	1:6:A:ARG:HA	1:9:A:ILE:HG12	2	0.93
(3,509)	1:14:A:ASP:HB2	1:19:A:SER:HB3	4	0.93
(3,461)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	5	0.93
(3,171)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	7	0.93
(3,103)	1:7:A:LEU:H	1:10:A:GLN:HB3	8	0.93
(3,103)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.93
(2,662)	1:6:A:ARG:HA	1:9:A:ILE:HG12	2	0.93
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	4	0.93
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	4	0.93
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	4	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	4	0.93
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	4	0.93
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	4	0.93
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	9	0.93
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	9	0.93
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	9	0.93
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	9	0.93
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	9	0.93
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	9	0.93
(2,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	4	0.93
(2,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	5	0.93
(2,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	5	0.93
(2,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	7	0.93
(2,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	8	0.93
(2,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.93
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG2	4	0.93
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG3	4	0.93
(1,631)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	9	0.93
(1,559)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	8	0.93
(1,559)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	10	0.93
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD11	10	0.93
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD12	10	0.93
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD13	10	0.93
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD21	10	0.93
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD22	10	0.93
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD23	10	0.93
(1,536)	1:8:A:TYR:HA	1:24:A:PRO:HG2	4	0.93
(1,536)	1:8:A:TYR:HA	1:24:A:PRO:HG2	8	0.93
(1,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	0.93
(1,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	0.93
(1,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	0.93
(1,122)	1:10:A:GLN:HA	1:10:A:GLN:HE21	1	0.93
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	1	0.92
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	1	0.92
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	1	0.92
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	1	0.92
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	1	0.92
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	1	0.92
(3,461)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	1	0.92
(3,461)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	6	0.92
(3,203)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	7	0.92
(3,148)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	5	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	1	0.92
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	1	0.92
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	1	0.92
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	1	0.92
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	1	0.92
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	1	0.92
(2,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	1	0.92
(2,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	6	0.92
(2,228)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	7	0.92
(2,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	5	0.92
(1,665)	1:10:A:GLN:HA	1:13:A:LYS:HD3	7	0.92
(1,559)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	1	0.92
(1,537)	1:8:A:TYR:HA	1:24:A:PRO:HG3	3	0.92
(1,537)	1:8:A:TYR:HA	1:24:A:PRO:HG3	9	0.92
(1,536)	1:8:A:TYR:HA	1:24:A:PRO:HG2	2	0.92
(1,319)	1:6:A:ARG:HA	1:6:A:ARG:HG2	2	0.92
(1,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	4	0.92
(1,287)	1:12:A:LEU:HD11	1:16:A:GLY:H	7	0.92
(1,287)	1:12:A:LEU:HD12	1:16:A:GLY:H	7	0.92
(1,287)	1:12:A:LEU:HD13	1:16:A:GLY:H	7	0.92
(1,271)	1:8:A:TYR:H	1:9:A:ILE:HB	6	0.92
(1,244)	1:8:A:TYR:HD1	1:9:A:ILE:H	1	0.92
(1,244)	1:8:A:TYR:HD2	1:9:A:ILE:H	1	0.92
(1,212)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	8	0.92
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	6	0.91
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	6	0.91
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	6	0.91
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	6	0.91
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	6	0.91
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	6	0.91
(4,9)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.91
(3,461)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	3	0.91
(3,461)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	7	0.91
(3,148)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	4	0.91
(3,145)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.91
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	6	0.91
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	6	0.91
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	6	0.91
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	6	0.91
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	6	0.91
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	6	0.91
(2,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	3	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	7	0.91
(2,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	4	0.91
(2,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.91
(2,110)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.91
(1,635)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	5	0.91
(1,635)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	5	0.91
(1,635)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	5	0.91
(1,568)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	5	0.91
(1,537)	1:8:A:TYR:HA	1:24:A:PRO:HG3	7	0.91
(1,536)	1:8:A:TYR:HA	1:24:A:PRO:HG2	6	0.91
(1,472)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	1	0.91
(1,271)	1:8:A:TYR:H	1:9:A:ILE:HB	9	0.91
(1,212)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	5	0.91
(1,170)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	0.91
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD11	6	0.91
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD12	6	0.91
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD13	6	0.91
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD21	6	0.91
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD22	6	0.91
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD23	6	0.91
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	9	0.9
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	9	0.9
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	9	0.9
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	9	0.9
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	9	0.9
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	9	0.9
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	9	0.9
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	9	0.9
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	9	0.9
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.9
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.9
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.9
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	10	0.9
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	10	0.9
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	10	0.9
(3,567)	1:15:A:GLY:HA3	1:18:A:SER:HB3	10	0.9
(3,550)	1:2:A:GLU:HB2	1:5:A:VAL:H	1	0.9
(3,461)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	8	0.9
(3,461)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	10	0.9
(3,145)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	5	0.9
(3,145)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	8	0.9
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	9	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	9	0.9
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	9	0.9
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	9	0.9
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	9	0.9
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	9	0.9
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	9	0.9
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	9	0.9
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	9	0.9
(2,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	10	0.9
(2,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	1	0.9
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.9
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.9
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.9
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	10	0.9
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	10	0.9
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	10	0.9
(2,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	8	0.9
(2,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	10	0.9
(2,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	5	0.9
(2,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	8	0.9
(1,588)	1:14:A:ASP:HB3	1:15:A:GLY:H	10	0.9
(1,567)	1:12:A:LEU:HA	1:16:A:GLY:HA2	3	0.9
(1,567)	1:12:A:LEU:HA	1:16:A:GLY:HA2	4	0.9
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	4	0.9
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	4	0.9
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	4	0.9
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	4	0.9
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	4	0.9
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	4	0.9
(1,537)	1:8:A:TYR:HA	1:24:A:PRO:HG3	8	0.9
(1,536)	1:8:A:TYR:HA	1:24:A:PRO:HG2	10	0.9
(1,319)	1:6:A:ARG:HA	1:6:A:ARG:HG2	1	0.9
(1,244)	1:8:A:TYR:HD1	1:9:A:ILE:H	9	0.9
(1,244)	1:8:A:TYR:HD2	1:9:A:ILE:H	9	0.9
(3,509)	1:14:A:ASP:HB2	1:19:A:SER:HB3	7	0.89
(3,461)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	9	0.89
(3,148)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	3	0.89
(3,103)	1:7:A:LEU:H	1:10:A:GLN:HB3	7	0.89
(2,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	7	0.89
(2,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	9	0.89
(2,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	3	0.89
(2,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	7	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG2	2	0.89
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG3	2	0.89
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG2	10	0.89
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG3	10	0.89
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	1	0.89
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	1	0.89
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	1	0.89
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	6	0.89
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	6	0.89
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	6	0.89
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	10	0.89
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	10	0.89
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	10	0.89
(1,559)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	5	0.89
(1,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	5	0.89
(1,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	7	0.89
(3,185)	1:23:A:PRO:HB3	1:25:A:CYS:H	1	0.88
(3,175)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	7	0.88
(3,175)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	7	0.88
(3,175)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	7	0.88
(3,163)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	6	0.88
(3,148)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	6	0.88
(3,146)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	4	0.88
(3,146)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	5	0.88
(2,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	1	0.88
(2,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	7	0.88
(2,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	7	0.88
(2,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	7	0.88
(2,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	6	0.88
(2,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	6	0.88
(2,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	4	0.88
(2,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	5	0.88
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	9	0.88
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	9	0.88
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	9	0.88
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	3	0.88
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	3	0.88
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	3	0.88
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	4	0.88
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	4	0.88
(1,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	4	0.88
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	4	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	4	0.88
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	4	0.88
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	4	0.88
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	4	0.88
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	4	0.88
(1,537)	1:8:A:TYR:HA	1:24:A:PRO:HG3	6	0.88
(1,536)	1:8:A:TYR:HA	1:24:A:PRO:HG2	7	0.88
(1,536)	1:8:A:TYR:HA	1:24:A:PRO:HG2	9	0.88
(1,472)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	7	0.88
(1,212)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	4	0.88
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	8	0.88
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	8	0.88
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	8	0.88
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	9	0.88
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	9	0.88
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	9	0.88
(1,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	7	0.88
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	1	0.87
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	1	0.87
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	1	0.87
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	1	0.87
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	1	0.87
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	1	0.87
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	1	0.87
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	1	0.87
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	1	0.87
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	8	0.87
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	8	0.87
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	8	0.87
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	8	0.87
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	8	0.87
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	8	0.87
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	8	0.87
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	8	0.87
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	8	0.87
(3,146)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	2	0.87
(3,146)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	7	0.87
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	1	0.87
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	1	0.87
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	1	0.87
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	1	0.87
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	1	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	1	0.87
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	1	0.87
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	1	0.87
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	1	0.87
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	8	0.87
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	8	0.87
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	8	0.87
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	8	0.87
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	8	0.87
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	8	0.87
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	8	0.87
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	8	0.87
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	8	0.87
(2,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	2	0.87
(2,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	7	0.87
(1,627)	1:14:A:ASP:HB3	1:19:A:SER:HB2	10	0.87
(1,568)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	7	0.87
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	8	0.87
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	8	0.87
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	8	0.87
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	8	0.87
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	8	0.87
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	8	0.87
(1,559)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	7	0.87
(1,536)	1:8:A:TYR:HA	1:24:A:PRO:HG2	3	0.87
(1,487)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	2	0.87
(1,472)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	4	0.87
(1,319)	1:6:A:ARG:HA	1:6:A:ARG:HG2	10	0.87
(1,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	2	0.87
(4,21)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	5	0.86
(4,21)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	5	0.86
(3,567)	1:15:A:GLY:HA3	1:18:A:SER:HB3	3	0.86
(3,163)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	9	0.86
(3,148)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	1	0.86
(2,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	3	0.86
(2,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	5	0.86
(2,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	5	0.86
(2,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	9	0.86
(2,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	1	0.86
(1,628)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	8	0.86
(1,627)	1:14:A:ASP:HB3	1:19:A:SER:HB2	3	0.86
(1,627)	1:14:A:ASP:HB3	1:19:A:SER:HB2	7	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	8	0.86
(1,567)	1:12:A:LEU:HA	1:16:A:GLY:HA2	5	0.86
(1,536)	1:8:A:TYR:HA	1:24:A:PRO:HG2	1	0.86
(1,536)	1:8:A:TYR:HA	1:24:A:PRO:HG2	5	0.86
(1,487)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	3	0.86
(1,487)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	6	0.86
(1,487)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	7	0.86
(1,487)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	9	0.86
(1,319)	1:6:A:ARG:HA	1:6:A:ARG:HG2	8	0.86
(1,244)	1:8:A:TYR:HD1	1:9:A:ILE:H	8	0.86
(1,244)	1:8:A:TYR:HD2	1:9:A:ILE:H	8	0.86
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	7	0.86
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	7	0.86
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	7	0.86
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	7	0.86
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	7	0.86
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	7	0.86
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	10	0.85
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	10	0.85
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	10	0.85
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	10	0.85
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	10	0.85
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	10	0.85
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	10	0.85
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	10	0.85
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	10	0.85
(4,21)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	3	0.85
(4,21)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	3	0.85
(4,21)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	6	0.85
(4,21)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	6	0.85
(4,21)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	8	0.85
(4,21)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	8	0.85
(3,611)	1:6:A:ARG:HA	1:9:A:ILE:HG12	5	0.85
(3,171)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	2	0.85
(3,163)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	8	0.85
(3,145)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	9	0.85
(2,662)	1:6:A:ARG:HA	1:9:A:ILE:HG12	5	0.85
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	10	0.85
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	10	0.85
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	10	0.85
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	10	0.85
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	10	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	10	0.85
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	10	0.85
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	10	0.85
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	10	0.85
(2,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	3	0.85
(2,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	3	0.85
(2,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	6	0.85
(2,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	6	0.85
(2,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	8	0.85
(2,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	8	0.85
(2,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	2	0.85
(2,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	8	0.85
(2,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	9	0.85
(1,543)	1:8:A:TYR:HA	1:24:A:PRO:HD2	10	0.85
(1,537)	1:8:A:TYR:HA	1:24:A:PRO:HG3	10	0.85
(1,498)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	9	0.85
(1,487)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	1	0.85
(1,487)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	8	0.85
(1,487)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.85
(1,472)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	3	0.85
(1,472)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	9	0.85
(1,271)	1:8:A:TYR:H	1:9:A:ILE:HB	1	0.85
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	6	0.84
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	6	0.84
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	6	0.84
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	6	0.84
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	6	0.84
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	6	0.84
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	6	0.84
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	6	0.84
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	6	0.84
(3,588)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	5	0.84
(3,509)	1:14:A:ASP:HB2	1:19:A:SER:HB3	9	0.84
(3,175)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.84
(3,175)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.84
(3,175)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.84
(3,146)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	3	0.84
(3,145)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	3	0.84
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	6	0.84
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	6	0.84
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	6	0.84
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	6	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	6	0.84
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	6	0.84
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	6	0.84
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	6	0.84
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	6	0.84
(2,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	5	0.84
(2,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	9	0.84
(2,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.84
(2,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.84
(2,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.84
(2,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	3	0.84
(2,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	3	0.84
(1,630)	1:2:A:GLU:HG2	1:5:A:VAL:HB	7	0.84
(1,630)	1:2:A:GLU:HG3	1:5:A:VAL:HB	7	0.84
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD21	10	0.84
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD22	10	0.84
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD23	10	0.84
(1,568)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	4	0.84
(1,568)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	9	0.84
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	1	0.84
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	1	0.84
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	1	0.84
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	1	0.84
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	1	0.84
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	1	0.84
(1,537)	1:8:A:TYR:HA	1:24:A:PRO:HG3	4	0.84
(1,498)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	10	0.84
(1,487)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	4	0.84
(1,487)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	5	0.84
(1,324)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	3	0.84
(1,234)	1:14:A:ASP:HB3	1:15:A:GLY:H	7	0.84
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	4	0.84
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	4	0.84
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	4	0.84
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.84
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.84
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.84
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	2	0.84
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	2	0.84
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	2	0.84
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	2	0.84
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	2	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	2	0.84
(1,22)	1:13:A:LYS:H	1:13:A:LYS:HD2	10	0.84
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	5	0.83
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	5	0.83
(4,40)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	5	0.83
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	5	0.83
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	5	0.83
(4,40)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	5	0.83
(3,509)	1:14:A:ASP:HB2	1:19:A:SER:HB3	1	0.83
(3,509)	1:14:A:ASP:HB2	1:19:A:SER:HB3	10	0.83
(3,148)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	10	0.83
(3,145)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	4	0.83
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	5	0.83
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	5	0.83
(2,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	5	0.83
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	5	0.83
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	5	0.83
(2,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	5	0.83
(2,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	1	0.83
(2,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	10	0.83
(2,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	10	0.83
(2,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	4	0.83
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	3	0.83
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	3	0.83
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	3	0.83
(1,628)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	10	0.83
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD21	1	0.83
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD22	1	0.83
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD23	1	0.83
(1,568)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	10	0.83
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	6	0.83
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	6	0.83
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	6	0.83
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	6	0.83
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	6	0.83
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	6	0.83
(1,543)	1:8:A:TYR:HA	1:24:A:PRO:HD2	1	0.83
(1,537)	1:8:A:TYR:HA	1:24:A:PRO:HG3	1	0.83
(1,537)	1:8:A:TYR:HA	1:24:A:PRO:HG3	2	0.83
(1,525)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	7	0.83
(1,525)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	7	0.83
(1,525)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	7	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,319)	1:6:A:ARG:HA	1:6:A:ARG:HG2	5	0.83
(1,244)	1:8:A:TYR:HD1	1:9:A:ILE:H	4	0.83
(1,244)	1:8:A:TYR:HD2	1:9:A:ILE:H	4	0.83
(1,202)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	2	0.83
(1,202)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	2	0.83
(1,59)	1:9:A:ILE:H	1:9:A:ILE:HG13	5	0.83
(3,509)	1:14:A:ASP:HB2	1:19:A:SER:HB3	6	0.82
(2,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	6	0.82
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	1	0.82
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	1	0.82
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	1	0.82
(1,628)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	6	0.82
(1,627)	1:14:A:ASP:HB3	1:19:A:SER:HB2	5	0.82
(1,625)	1:8:A:TYR:HB2	1:25:A:CYS:HB3	1	0.82
(1,625)	1:8:A:TYR:HB3	1:25:A:CYS:HB3	1	0.82
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD21	6	0.82
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD22	6	0.82
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD23	6	0.82
(1,568)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	3	0.82
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD11	6	0.82
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD12	6	0.82
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD13	6	0.82
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD21	6	0.82
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD22	6	0.82
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD23	6	0.82
(1,543)	1:8:A:TYR:HA	1:24:A:PRO:HD2	4	0.82
(1,543)	1:8:A:TYR:HA	1:24:A:PRO:HD2	6	0.82
(1,543)	1:8:A:TYR:HA	1:24:A:PRO:HD2	9	0.82
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB2	2	0.82
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB3	2	0.82
(1,498)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	8	0.82
(1,390)	1:13:A:LYS:HA	1:13:A:LYS:HD2	2	0.82
(1,314)	1:6:A:ARG:HA	1:6:A:ARG:HD3	2	0.82
(1,281)	1:24:A:PRO:HG2	1:25:A:CYS:H	8	0.82
(1,271)	1:8:A:TYR:H	1:9:A:ILE:HB	10	0.82
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	3	0.82
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	3	0.82
(3,489)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	1	0.81
(3,489)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	0.81
(3,489)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	0.81
(3,185)	1:23:A:PRO:HB3	1:25:A:CYS:H	10	0.81
(3,145)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	7	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	1	0.81
(2,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	0.81
(2,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	0.81
(2,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	10	0.81
(2,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	7	0.81
(1,628)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	1	0.81
(1,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	8	0.81
(1,588)	1:14:A:ASP:HB3	1:15:A:GLY:H	4	0.81
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD21	3	0.81
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD22	3	0.81
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD23	3	0.81
(1,543)	1:8:A:TYR:HA	1:24:A:PRO:HD2	5	0.81
(1,537)	1:8:A:TYR:HA	1:24:A:PRO:HG3	5	0.81
(1,498)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	3	0.81
(1,472)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	5	0.81
(1,472)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	8	0.81
(1,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	6	0.81
(1,281)	1:24:A:PRO:HG2	1:25:A:CYS:H	9	0.81
(1,234)	1:14:A:ASP:HB3	1:15:A:GLY:H	10	0.81
(1,202)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	5	0.81
(1,202)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	5	0.81
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	1	0.81
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	1	0.81
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	1	0.81
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	3	0.81
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	3	0.81
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	3	0.81
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	6	0.81
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	6	0.81
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	6	0.81
(4,21)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	10	0.8
(4,21)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	10	0.8
(3,588)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	2	0.8
(3,550)	1:2:A:GLU:HB2	1:5:A:VAL:H	9	0.8
(3,489)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	0.8
(3,489)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	0.8
(3,163)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.8
(3,145)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	1	0.8
(2,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	2	0.8
(2,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	9	0.8
(2,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	0.8
(2,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	10	0.8
(2,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	10	0.8
(2,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.8
(2,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	1	0.8
(1,627)	1:14:A:ASP:HB3	1:19:A:SER:HB2	6	0.8
(1,601)	1:8:A:TYR:HD1	1:25:A:CYS:HB3	7	0.8
(1,601)	1:8:A:TYR:HD2	1:25:A:CYS:HB3	7	0.8
(1,588)	1:14:A:ASP:HB3	1:15:A:GLY:H	6	0.8
(1,472)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	10	0.8
(1,246)	1:8:A:TYR:HD1	1:25:A:CYS:H	2	0.8
(1,246)	1:8:A:TYR:HD2	1:25:A:CYS:H	2	0.8
(1,202)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	7	0.8
(1,202)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	7	0.8
(1,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	8	0.8
(1,59)	1:9:A:ILE:H	1:9:A:ILE:HG13	4	0.8
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	5	0.8
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	5	0.8
(1,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	5	0.8
(3,489)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	0.79
(3,489)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	0.79
(3,146)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	1	0.79
(3,146)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	6	0.79
(2,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	0.79
(2,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	0.79
(2,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	1	0.79
(2,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	6	0.79
(1,668)	1:1:A:GLU:HA	1:1:A:GLU:HB3	7	0.79
(1,635)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	7	0.79
(1,635)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	7	0.79
(1,635)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	7	0.79
(1,577)	1:20:A:GLY:H	1:21:A:ARG:H	9	0.79
(1,543)	1:8:A:TYR:HA	1:24:A:PRO:HD2	8	0.79
(1,498)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	1	0.79
(1,498)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	7	0.79
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	2	0.79
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	2	0.79
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	2	0.79
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	2	0.79
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG2	6	0.79
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG3	6	0.79
(1,212)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	9	0.79
(1,59)	1:9:A:ILE:H	1:9:A:ILE:HG13	6	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,23)	1:11:A:TRP:HE3	1:12:A:LEU:HG	1	0.78
(3,489)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.78
(3,163)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	4	0.78
(3,163)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	5	0.78
(3,146)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.78
(3,96)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.78
(3,96)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.78
(3,96)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.78
(2,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.78
(2,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	1	0.78
(2,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	4	0.78
(2,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	5	0.78
(2,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.78
(2,104)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.78
(2,104)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.78
(2,104)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.78
(1,668)	1:1:A:GLU:HA	1:1:A:GLU:HB3	10	0.78
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	1	0.78
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	1	0.78
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	1	0.78
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	10	0.78
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	10	0.78
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	10	0.78
(1,634)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	4	0.78
(1,634)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	4	0.78
(1,634)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	4	0.78
(1,628)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	3	0.78
(1,628)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	7	0.78
(1,627)	1:14:A:ASP:HB3	1:19:A:SER:HB2	2	0.78
(1,627)	1:14:A:ASP:HB3	1:19:A:SER:HB2	4	0.78
(1,588)	1:14:A:ASP:HB3	1:15:A:GLY:H	2	0.78
(1,447)	1:22:A:PRO:HA	1:22:A:PRO:HB3	3	0.78
(1,269)	1:7:A:LEU:HG	1:8:A:TYR:H	6	0.78
(1,246)	1:8:A:TYR:HD1	1:25:A:CYS:H	8	0.78
(1,246)	1:8:A:TYR:HD2	1:25:A:CYS:H	8	0.78
(1,212)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	2	0.78
(1,59)	1:9:A:ILE:H	1:9:A:ILE:HG13	3	0.78
(1,59)	1:9:A:ILE:H	1:9:A:ILE:HG13	9	0.78
(4,23)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	0.77
(4,23)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	0.77
(4,21)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	9	0.77
(4,21)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	9	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,611)	1:6:A:ARG:HA	1:9:A:ILE:HG12	7	0.77
(3,163)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	7	0.77
(3,148)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	9	0.77
(3,146)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	9	0.77
(2,662)	1:6:A:ARG:HA	1:9:A:ILE:HG12	7	0.77
(2,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	0.77
(2,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	0.77
(2,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	9	0.77
(2,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	9	0.77
(2,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	7	0.77
(2,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	9	0.77
(2,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	9	0.77
(1,630)	1:2:A:GLU:HG2	1:5:A:VAL:HB	3	0.77
(1,630)	1:2:A:GLU:HG3	1:5:A:VAL:HB	3	0.77
(1,601)	1:8:A:TYR:HD1	1:25:A:CYS:HB3	1	0.77
(1,601)	1:8:A:TYR:HD2	1:25:A:CYS:HB3	1	0.77
(1,580)	1:5:A:VAL:HG11	1:9:A:ILE:H	3	0.77
(1,580)	1:5:A:VAL:HG12	1:9:A:ILE:H	3	0.77
(1,580)	1:5:A:VAL:HG13	1:9:A:ILE:H	3	0.77
(1,568)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	1	0.77
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB2	5	0.77
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB3	5	0.77
(1,498)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	6	0.77
(1,472)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	6	0.77
(1,447)	1:22:A:PRO:HA	1:22:A:PRO:HB3	1	0.77
(1,447)	1:22:A:PRO:HA	1:22:A:PRO:HB3	2	0.77
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	1	0.77
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	1	0.77
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	1	0.77
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	1	0.77
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG2	7	0.77
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG3	7	0.77
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG2	10	0.77
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG3	10	0.77
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	10	0.77
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	10	0.77
(1,207)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	2	0.77
(1,194)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	7	0.77
(1,194)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	7	0.77
(1,194)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	7	0.77
(1,194)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	7	0.77
(1,194)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	7	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	7	0.77
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	5	0.77
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	5	0.77
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	5	0.77
(1,115)	1:2:A:GLU:HB3	1:5:A:VAL:H	6	0.77
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	8	0.77
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	8	0.77
(1,59)	1:9:A:ILE:H	1:9:A:ILE:HG13	8	0.77
(1,59)	1:9:A:ILE:H	1:9:A:ILE:HG13	10	0.77
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	4	0.76
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	4	0.76
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	4	0.76
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	4	0.76
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	4	0.76
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	4	0.76
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	4	0.76
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	4	0.76
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	4	0.76
(3,550)	1:2:A:GLU:HB2	1:5:A:VAL:H	10	0.76
(3,163)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	3	0.76
(3,148)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	8	0.76
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	4	0.76
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	4	0.76
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	4	0.76
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	4	0.76
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	4	0.76
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	4	0.76
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	4	0.76
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	4	0.76
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	4	0.76
(2,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	10	0.76
(2,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	3	0.76
(2,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	8	0.76
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	6	0.76
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	6	0.76
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	6	0.76
(1,600)	1:11:A:TRP:HZ3	1:17:A:PRO:HD3	8	0.76
(1,600)	1:11:A:TRP:HZ3	1:17:A:PRO:HD3	9	0.76
(1,568)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	6	0.76
(1,543)	1:8:A:TYR:HA	1:24:A:PRO:HD2	3	0.76
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	3	0.76
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	3	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	3	0.76
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	3	0.76
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	5	0.76
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	5	0.76
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	5	0.76
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	5	0.76
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	7	0.76
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	7	0.76
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	7	0.76
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	7	0.76
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	8	0.76
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	8	0.76
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	8	0.76
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	8	0.76
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	9	0.76
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	9	0.76
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	9	0.76
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	9	0.76
(1,281)	1:24:A:PRO:HG2	1:25:A:CYS:H	4	0.76
(1,271)	1:8:A:TYR:H	1:9:A:ILE:HB	2	0.76
(1,269)	1:7:A:LEU:HG	1:8:A:TYR:H	9	0.76
(1,194)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	2	0.76
(1,194)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	2	0.76
(1,194)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	2	0.76
(1,194)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	2	0.76
(1,194)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	2	0.76
(1,194)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	2	0.76
(3,550)	1:2:A:GLU:HB2	1:5:A:VAL:H	7	0.75
(3,203)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	5	0.75
(2,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	7	0.75
(2,228)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	5	0.75
(1,668)	1:1:A:GLU:HA	1:1:A:GLU:HB3	2	0.75
(1,668)	1:1:A:GLU:HA	1:1:A:GLU:HB3	8	0.75
(1,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	2	0.75
(1,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	2	0.75
(1,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	2	0.75
(1,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	2	0.75
(1,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	2	0.75
(1,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	2	0.75
(1,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	2	0.75
(1,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	2	0.75
(1,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	2	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	7	0.75
(1,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	7	0.75
(1,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	7	0.75
(1,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	7	0.75
(1,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	7	0.75
(1,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	7	0.75
(1,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	7	0.75
(1,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	7	0.75
(1,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	7	0.75
(1,627)	1:14:A:ASP:HB3	1:19:A:SER:HB2	1	0.75
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD21	4	0.75
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD22	4	0.75
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD23	4	0.75
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD21	5	0.75
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD22	5	0.75
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD23	5	0.75
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	1	0.75
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	1	0.75
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	1	0.75
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	1	0.75
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	1	0.75
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	1	0.75
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	9	0.75
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	9	0.75
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	9	0.75
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	9	0.75
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	9	0.75
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	9	0.75
(1,543)	1:8:A:TYR:HA	1:24:A:PRO:HD2	2	0.75
(1,498)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	4	0.75
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	6	0.75
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	6	0.75
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	10	0.75
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	10	0.75
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	4	0.75
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	4	0.75
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	4	0.75
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	4	0.75
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	6	0.75
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	6	0.75
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	6	0.75
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	6	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	0.75
(1,397)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	0.75
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	10	0.75
(1,397)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	10	0.75
(1,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	9	0.75
(1,267)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	3	0.75
(1,246)	1:8:A:TYR:HD1	1:25:A:CYS:H	5	0.75
(1,246)	1:8:A:TYR:HD2	1:25:A:CYS:H	5	0.75
(1,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	2	0.75
(1,59)	1:9:A:ILE:H	1:9:A:ILE:HG13	1	0.75
(1,59)	1:9:A:ILE:H	1:9:A:ILE:HG13	7	0.75
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	5	0.74
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	5	0.74
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	5	0.74
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	5	0.74
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	5	0.74
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	5	0.74
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	5	0.74
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	5	0.74
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	5	0.74
(3,203)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	2	0.74
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	5	0.74
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	5	0.74
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	5	0.74
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	5	0.74
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	5	0.74
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	5	0.74
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	5	0.74
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	5	0.74
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	5	0.74
(2,228)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	2	0.74
(1,625)	1:8:A:TYR:HB2	1:25:A:CYS:HB3	10	0.74
(1,625)	1:8:A:TYR:HB3	1:25:A:CYS:HB3	10	0.74
(1,623)	1:5:A:VAL:HA	1:25:A:CYS:HB2	9	0.74
(1,568)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	2	0.74
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	9	0.74
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	9	0.74
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	9	0.74
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	9	0.74
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	9	0.74
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	9	0.74
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB2	6	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB3	6	0.74
(1,498)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	5	0.74
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	4	0.74
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	4	0.74
(1,59)	1:9:A:ILE:H	1:9:A:ILE:HG13	2	0.74
(3,550)	1:2:A:GLU:HB2	1:5:A:VAL:H	6	0.73
(3,163)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	1	0.73
(3,146)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	8	0.73
(2,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	6	0.73
(2,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	1	0.73
(2,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	8	0.73
(1,668)	1:1:A:GLU:HA	1:1:A:GLU:HB3	4	0.73
(1,665)	1:10:A:GLN:HA	1:13:A:LYS:HD3	1	0.73
(1,628)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	4	0.73
(1,588)	1:14:A:ASP:HB3	1:15:A:GLY:H	1	0.73
(1,588)	1:14:A:ASP:HB3	1:15:A:GLY:H	8	0.73
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	10	0.73
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	10	0.73
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	10	0.73
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	10	0.73
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	10	0.73
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	10	0.73
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	7	0.73
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	7	0.73
(1,433)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	8	0.73
(1,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	8	0.73
(1,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	5	0.73
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	8	0.72
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	8	0.72
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	8	0.72
(3,550)	1:2:A:GLU:HB2	1:5:A:VAL:H	5	0.72
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	8	0.72
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	8	0.72
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	8	0.72
(2,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	5	0.72
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	1	0.72
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	1	0.72
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	1	0.72
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	4	0.72
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	4	0.72
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	4	0.72
(1,628)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	5	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:20:A:GLY:H	1:21:A:ARG:H	3	0.72
(1,577)	1:20:A:GLY:H	1:21:A:ARG:H	6	0.72
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB2	8	0.72
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB3	8	0.72
(1,543)	1:8:A:TYR:HA	1:24:A:PRO:HD2	7	0.72
(1,447)	1:22:A:PRO:HA	1:22:A:PRO:HB3	7	0.72
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG2	3	0.72
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG3	3	0.72
(1,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	2	0.72
(1,281)	1:24:A:PRO:HG2	1:25:A:CYS:H	7	0.72
(1,267)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	9	0.72
(1,246)	1:8:A:TYR:HD1	1:25:A:CYS:H	4	0.72
(1,246)	1:8:A:TYR:HD2	1:25:A:CYS:H	4	0.72
(1,234)	1:14:A:ASP:HB3	1:15:A:GLY:H	4	0.72
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	6	0.72
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	6	0.72
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	2	0.71
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	2	0.71
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	2	0.71
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	2	0.71
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	2	0.71
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	2	0.71
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	2	0.71
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	2	0.71
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	2	0.71
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	7	0.71
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	7	0.71
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	7	0.71
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	7	0.71
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	7	0.71
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	7	0.71
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	7	0.71
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	7	0.71
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	7	0.71
(3,561)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.71
(3,561)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.71
(3,489)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	0.71
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	2	0.71
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	2	0.71
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	2	0.71
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	2	0.71
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	2	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	2	0.71
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	2	0.71
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	2	0.71
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	2	0.71
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	7	0.71
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	7	0.71
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	7	0.71
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	7	0.71
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	7	0.71
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	7	0.71
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	7	0.71
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	7	0.71
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	7	0.71
(2,604)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.71
(2,604)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.71
(2,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	0.71
(1,668)	1:1:A:GLU:HA	1:1:A:GLU:HB3	3	0.71
(1,668)	1:1:A:GLU:HA	1:1:A:GLU:HB3	9	0.71
(1,665)	1:10:A:GLN:HA	1:13:A:LYS:HD3	4	0.71
(1,665)	1:10:A:GLN:HA	1:13:A:LYS:HD3	5	0.71
(1,661)	1:9:A:ILE:HA	1:12:A:LEU:HB2	1	0.71
(1,610)	1:15:A:GLY:HA3	1:19:A:SER:HB3	8	0.71
(1,577)	1:20:A:GLY:H	1:21:A:ARG:H	5	0.71
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB2	2	0.71
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB3	2	0.71
(1,548)	1:14:A:ASP:HB3	1:19:A:SER:HB3	8	0.71
(1,447)	1:22:A:PRO:HA	1:22:A:PRO:HB3	4	0.71
(1,447)	1:22:A:PRO:HA	1:22:A:PRO:HB3	5	0.71
(1,447)	1:22:A:PRO:HA	1:22:A:PRO:HB3	6	0.71
(1,447)	1:22:A:PRO:HA	1:22:A:PRO:HB3	8	0.71
(1,447)	1:22:A:PRO:HA	1:22:A:PRO:HB3	9	0.71
(1,447)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.71
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG2	4	0.71
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG3	4	0.71
(1,271)	1:8:A:TYR:H	1:9:A:ILE:HB	5	0.71
(1,267)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	2	0.71
(1,212)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	10	0.71
(1,115)	1:2:A:GLU:HB3	1:5:A:VAL:H	7	0.71
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	9	0.71
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	9	0.71
(3,561)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	1	0.7
(3,561)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	1	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,203)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	4	0.7
(3,145)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	2	0.7
(2,604)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	1	0.7
(2,604)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	1	0.7
(2,228)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	4	0.7
(2,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	2	0.7
(1,631)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	6	0.7
(1,601)	1:8:A:TYR:HD1	1:25:A:CYS:HB3	10	0.7
(1,601)	1:8:A:TYR:HD2	1:25:A:CYS:HB3	10	0.7
(1,600)	1:11:A:TRP:HZ3	1:17:A:PRO:HD3	10	0.7
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB2	9	0.7
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB3	9	0.7
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	2	0.7
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	2	0.7
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	2	0.7
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	7	0.7
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	7	0.7
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	7	0.7
(1,294)	1:2:A:GLU:HA	1:2:A:GLU:HB3	4	0.7
(1,267)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	5	0.7
(1,244)	1:8:A:TYR:HD1	1:9:A:ILE:H	5	0.7
(1,244)	1:8:A:TYR:HD2	1:9:A:ILE:H	5	0.7
(1,234)	1:14:A:ASP:HB3	1:15:A:GLY:H	6	0.7
(1,212)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	6	0.7
(1,176)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	4	0.7
(1,176)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	4	0.7
(1,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	1	0.7
(1,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	4	0.7
(1,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	8	0.7
(1,153)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	8	0.7
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	3	0.69
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	3	0.69
(4,50)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	3	0.69
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	3	0.69
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	3	0.69
(4,50)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	3	0.69
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	3	0.69
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	3	0.69
(4,50)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	3	0.69
(3,178)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	7	0.69
(3,178)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	7	0.69
(3,178)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	7	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,178)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	7	0.69
(3,178)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	7	0.69
(3,178)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	7	0.69
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	3	0.69
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	3	0.69
(2,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	3	0.69
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	3	0.69
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	3	0.69
(2,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	3	0.69
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	3	0.69
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	3	0.69
(2,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	3	0.69
(2,197)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	7	0.69
(2,197)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	7	0.69
(2,197)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	7	0.69
(2,197)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	7	0.69
(2,197)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	7	0.69
(2,197)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	7	0.69
(1,668)	1:1:A:GLU:HA	1:1:A:GLU:HB3	5	0.69
(1,668)	1:1:A:GLU:HA	1:1:A:GLU:HB3	6	0.69
(1,661)	1:9:A:ILE:HA	1:12:A:LEU:HB2	5	0.69
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	9	0.69
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	9	0.69
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	9	0.69
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB2	3	0.69
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB3	3	0.69
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB2	4	0.69
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB3	4	0.69
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG2	8	0.69
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG3	8	0.69
(1,267)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	4	0.69
(1,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	3	0.69
(1,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	6	0.69
(1,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	7	0.69
(1,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	9	0.69
(1,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	0.69
(4,23)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	0.68
(3,561)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	2	0.68
(3,561)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	2	0.68
(3,185)	1:23:A:PRO:HB3	1:25:A:CYS:H	3	0.68
(3,185)	1:23:A:PRO:HB3	1:25:A:CYS:H	4	0.68
(3,178)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,178)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	2	0.68
(3,178)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	2	0.68
(3,178)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	2	0.68
(3,178)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	2	0.68
(3,178)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	2	0.68
(2,604)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	2	0.68
(2,604)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	2	0.68
(2,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	0.68
(2,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	3	0.68
(2,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	4	0.68
(2,197)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	2	0.68
(2,197)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	2	0.68
(2,197)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	2	0.68
(2,197)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	2	0.68
(2,197)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	2	0.68
(2,197)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	2	0.68
(1,661)	1:9:A:ILE:HA	1:12:A:LEU:HB2	9	0.68
(1,661)	1:9:A:ILE:HA	1:12:A:LEU:HB2	10	0.68
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	3	0.68
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	3	0.68
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	3	0.68
(1,634)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	7	0.68
(1,634)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	7	0.68
(1,634)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	7	0.68
(1,625)	1:8:A:TYR:HB2	1:25:A:CYS:HB3	2	0.68
(1,625)	1:8:A:TYR:HB3	1:25:A:CYS:HB3	2	0.68
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB2	1	0.68
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB3	1	0.68
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	5	0.68
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	5	0.68
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	9	0.68
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	9	0.68
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG2	5	0.68
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG3	5	0.68
(1,324)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	1	0.68
(1,322)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	7	0.68
(1,234)	1:14:A:ASP:HB3	1:15:A:GLY:H	2	0.68
(1,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	10	0.68
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	5	0.68
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	5	0.68
(1,75)	1:19:A:SER:H	1:19:A:SER:HB3	8	0.68
(4,47)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	9	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,47)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	9	0.67
(4,47)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	9	0.67
(3,550)	1:2:A:GLU:HB2	1:5:A:VAL:H	2	0.67
(3,489)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	0.67
(2,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	9	0.67
(2,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	9	0.67
(2,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	9	0.67
(2,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	2	0.67
(2,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	0.67
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	6	0.67
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	6	0.67
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	6	0.67
(1,635)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	8	0.67
(1,635)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	8	0.67
(1,635)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	8	0.67
(1,600)	1:11:A:TRP:HZ3	1:17:A:PRO:HD3	1	0.67
(1,580)	1:5:A:VAL:HG11	1:9:A:ILE:H	4	0.67
(1,580)	1:5:A:VAL:HG12	1:9:A:ILE:H	4	0.67
(1,580)	1:5:A:VAL:HG13	1:9:A:ILE:H	4	0.67
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB2	10	0.67
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB3	10	0.67
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	1	0.67
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	1	0.67
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	3	0.67
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	3	0.67
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	4	0.67
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	4	0.67
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	6	0.67
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	6	0.67
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	7	0.67
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	7	0.67
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	10	0.67
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	10	0.67
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG2	9	0.67
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG3	9	0.67
(1,269)	1:7:A:LEU:HG	1:8:A:TYR:H	1	0.67
(1,267)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	1	0.67
(1,212)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	3	0.67
(1,212)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	7	0.67
(1,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	6	0.67
(1,115)	1:2:A:GLU:HB3	1:5:A:VAL:H	9	0.67
(1,115)	1:2:A:GLU:HB3	1:5:A:VAL:H	10	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,23)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.66
(3,561)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	3	0.66
(3,561)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	3	0.66
(3,561)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	6	0.66
(3,561)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	6	0.66
(3,40)	1:2:A:GLU:HG3	1:6:A:ARG:H	4	0.66
(2,604)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	3	0.66
(2,604)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	3	0.66
(2,604)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	6	0.66
(2,604)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	6	0.66
(2,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.66
(2,46)	1:2:A:GLU:HG3	1:6:A:ARG:H	4	0.66
(1,661)	1:9:A:ILE:HA	1:12:A:LEU:HB2	6	0.66
(1,661)	1:9:A:ILE:HA	1:12:A:LEU:HB2	8	0.66
(1,588)	1:14:A:ASP:HB3	1:15:A:GLY:H	3	0.66
(1,541)	1:4:A:CYS:HA	1:7:A:LEU:HB2	6	0.66
(1,433)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	4	0.66
(1,324)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	8	0.66
(1,319)	1:6:A:ARG:HA	1:6:A:ARG:HG2	4	0.66
(1,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	3	0.66
(1,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	1	0.66
(1,153)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	9	0.66
(1,115)	1:2:A:GLU:HB3	1:5:A:VAL:H	2	0.66
(1,64)	1:18:A:SER:H	1:18:A:SER:HB2	1	0.66
(3,575)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	1	0.65
(3,561)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	9	0.65
(3,561)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	9	0.65
(3,203)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	10	0.65
(2,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	1	0.65
(2,604)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	9	0.65
(2,604)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	9	0.65
(2,228)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	10	0.65
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	5	0.65
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	5	0.65
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	5	0.65
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG21	3	0.65
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG22	3	0.65
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG23	3	0.65
(1,634)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	9	0.65
(1,634)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	9	0.65
(1,634)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	9	0.65
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	7	0.65
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	7	0.65
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	7	0.65
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	7	0.65
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	7	0.65
(1,600)	1:11:A:TRP:HZ3	1:17:A:PRO:HD3	6	0.65
(1,588)	1:14:A:ASP:HB3	1:15:A:GLY:H	5	0.65
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	7	0.65
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	7	0.65
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	7	0.65
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	7	0.65
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	7	0.65
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	7	0.65
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	10	0.65
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	10	0.65
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	10	0.65
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	10	0.65
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	10	0.65
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	10	0.65
(1,498)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	2	0.65
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	2	0.65
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	2	0.65
(1,433)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	2	0.65
(1,433)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	3	0.65
(1,421)	1:18:A:SER:HA	1:18:A:SER:HB3	6	0.65
(1,421)	1:18:A:SER:HA	1:18:A:SER:HB3	10	0.65
(1,346)	1:9:A:ILE:HA	1:9:A:ILE:HG12	7	0.65
(1,323)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	2	0.65
(1,323)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	10	0.65
(1,267)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	6	0.65
(1,267)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	8	0.65
(1,267)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	10	0.65
(1,176)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	1	0.65
(1,176)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	1	0.65
(1,153)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	10	0.65
(1,64)	1:18:A:SER:H	1:18:A:SER:HB2	7	0.65
(4,37)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	3	0.64
(4,37)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	5	0.64
(4,37)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	7	0.64
(3,575)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	3	0.64
(3,96)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.64
(2,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	3	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,508)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	3	0.64
(2,508)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	5	0.64
(2,508)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	7	0.64
(2,104)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.64
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	4	0.64
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	4	0.64
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	4	0.64
(1,634)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	6	0.64
(1,634)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	6	0.64
(1,634)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	6	0.64
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD21	9	0.64
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD22	9	0.64
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD23	9	0.64
(1,442)	1:22:A:PRO:HA	1:22:A:PRO:HD3	10	0.64
(1,421)	1:18:A:SER:HA	1:18:A:SER:HB3	3	0.64
(1,267)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	7	0.64
(1,234)	1:14:A:ASP:HB3	1:15:A:GLY:H	1	0.64
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	1	0.64
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	1	0.64
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	2	0.64
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	2	0.64
(1,176)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	5	0.64
(1,176)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	5	0.64
(1,156)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	2	0.64
(1,115)	1:2:A:GLU:HB3	1:5:A:VAL:H	1	0.64
(1,18)	1:6:A:ARG:H	1:6:A:ARG:HG2	7	0.64
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	3	0.63
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	3	0.63
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	3	0.63
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	3	0.63
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	3	0.63
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	3	0.63
(4,37)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	1	0.63
(4,37)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	2	0.63
(4,37)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	4	0.63
(4,37)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	6	0.63
(4,37)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	8	0.63
(4,37)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	9	0.63
(4,37)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	10	0.63
(3,613)	1:10:A:GLN:HA	1:13:A:LYS:HD2	2	0.63
(3,575)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	2	0.63
(3,561)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	4	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,561)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	4	0.63
(3,561)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	5	0.63
(3,561)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	5	0.63
(3,492)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	3	0.63
(3,203)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	3	0.63
(2,664)	1:10:A:GLN:HA	1:13:A:LYS:HD2	2	0.63
(2,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	2	0.63
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	3	0.63
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	3	0.63
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	3	0.63
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	3	0.63
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	3	0.63
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	3	0.63
(2,604)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	4	0.63
(2,604)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	4	0.63
(2,604)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	5	0.63
(2,604)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	5	0.63
(2,530)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	3	0.63
(2,508)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	1	0.63
(2,508)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	2	0.63
(2,508)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	4	0.63
(2,508)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	6	0.63
(2,508)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	8	0.63
(2,508)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	9	0.63
(2,508)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	10	0.63
(2,228)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	3	0.63
(1,661)	1:9:A:ILE:HA	1:12:A:LEU:HB2	3	0.63
(1,658)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	3	0.63
(1,658)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	3	0.63
(1,658)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	3	0.63
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	6	0.63
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	6	0.63
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	6	0.63
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	7	0.63
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	7	0.63
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	7	0.63
(1,629)	1:2:A:GLU:HG3	1:5:A:VAL:HB	9	0.63
(1,600)	1:11:A:TRP:HZ3	1:17:A:PRO:HD3	3	0.63
(1,467)	1:23:A:PRO:HA	1:23:A:PRO:HB3	2	0.63
(1,442)	1:22:A:PRO:HA	1:22:A:PRO:HD3	6	0.63
(1,442)	1:22:A:PRO:HA	1:22:A:PRO:HD3	9	0.63
(1,346)	1:9:A:ILE:HA	1:9:A:ILE:HG12	2	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,319)	1:6:A:ARG:HA	1:6:A:ARG:HG2	9	0.63
(1,271)	1:8:A:TYR:H	1:9:A:ILE:HB	7	0.63
(1,246)	1:8:A:TYR:HD1	1:25:A:CYS:H	7	0.63
(1,246)	1:8:A:TYR:HD2	1:25:A:CYS:H	7	0.63
(1,234)	1:14:A:ASP:HB3	1:15:A:GLY:H	8	0.63
(1,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	9	0.63
(1,153)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	1	0.63
(1,22)	1:13:A:LYS:H	1:13:A:LYS:HD2	4	0.63
(3,561)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	7	0.62
(3,561)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	7	0.62
(3,492)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	2	0.62
(2,604)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	7	0.62
(2,604)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	7	0.62
(2,530)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	2	0.62
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG2	7	0.62
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG3	7	0.62
(1,661)	1:9:A:ILE:HA	1:12:A:LEU:HB2	4	0.62
(1,629)	1:2:A:GLU:HG3	1:5:A:VAL:HB	1	0.62
(1,580)	1:5:A:VAL:HG11	1:9:A:ILE:H	8	0.62
(1,580)	1:5:A:VAL:HG12	1:9:A:ILE:H	8	0.62
(1,580)	1:5:A:VAL:HG13	1:9:A:ILE:H	8	0.62
(1,580)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	0.62
(1,580)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	0.62
(1,580)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	0.62
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB2	7	0.62
(1,549)	1:5:A:VAL:HA	1:8:A:TYR:HB3	7	0.62
(1,467)	1:23:A:PRO:HA	1:23:A:PRO:HB3	6	0.62
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	8	0.62
(1,438)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	8	0.62
(1,433)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	5	0.62
(1,433)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	9	0.62
(1,403)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	1	0.62
(1,403)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	2	0.62
(1,403)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	3	0.62
(1,403)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	5	0.62
(1,403)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	9	0.62
(1,324)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	2	0.62
(1,323)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	5	0.62
(1,246)	1:8:A:TYR:HD1	1:25:A:CYS:H	6	0.62
(1,246)	1:8:A:TYR:HD2	1:25:A:CYS:H	6	0.62
(1,199)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	2	0.62
(1,199)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	2	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	2	0.62
(1,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	1	0.62
(1,143)	1:23:A:PRO:HB2	1:25:A:CYS:H	7	0.62
(1,64)	1:18:A:SER:H	1:18:A:SER:HB2	4	0.62
(1,64)	1:18:A:SER:H	1:18:A:SER:HB2	8	0.62
(3,561)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	8	0.61
(3,561)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	8	0.61
(3,39)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	1	0.61
(3,39)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	3	0.61
(2,604)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	8	0.61
(2,604)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	8	0.61
(2,45)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	1	0.61
(2,45)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	3	0.61
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG21	6	0.61
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG22	6	0.61
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG23	6	0.61
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	5	0.61
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	5	0.61
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	5	0.61
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	5	0.61
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	5	0.61
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	5	0.61
(1,600)	1:11:A:TRP:HZ3	1:17:A:PRO:HD3	4	0.61
(1,580)	1:5:A:VAL:HG11	1:9:A:ILE:H	6	0.61
(1,580)	1:5:A:VAL:HG12	1:9:A:ILE:H	6	0.61
(1,580)	1:5:A:VAL:HG13	1:9:A:ILE:H	6	0.61
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	2	0.61
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	2	0.61
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	2	0.61
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	2	0.61
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	2	0.61
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	2	0.61
(1,477)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	2	0.61
(1,467)	1:23:A:PRO:HA	1:23:A:PRO:HB3	1	0.61
(1,467)	1:23:A:PRO:HA	1:23:A:PRO:HB3	3	0.61
(1,467)	1:23:A:PRO:HA	1:23:A:PRO:HB3	4	0.61
(1,467)	1:23:A:PRO:HA	1:23:A:PRO:HB3	7	0.61
(1,467)	1:23:A:PRO:HA	1:23:A:PRO:HB3	8	0.61
(1,467)	1:23:A:PRO:HA	1:23:A:PRO:HB3	9	0.61
(1,467)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.61
(1,442)	1:22:A:PRO:HA	1:22:A:PRO:HD3	4	0.61
(1,442)	1:22:A:PRO:HA	1:22:A:PRO:HD3	7	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,403)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	4	0.61
(1,403)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	6	0.61
(1,403)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	7	0.61
(1,403)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.61
(1,319)	1:6:A:ARG:HA	1:6:A:ARG:HG2	3	0.61
(1,281)	1:24:A:PRO:HG2	1:25:A:CYS:H	2	0.61
(1,281)	1:24:A:PRO:HG2	1:25:A:CYS:H	5	0.61
(1,269)	1:7:A:LEU:HG	1:8:A:TYR:H	10	0.61
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	8	0.61
(1,176)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	2	0.61
(1,176)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	2	0.61
(1,176)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	6	0.61
(1,176)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	6	0.61
(1,176)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	10	0.61
(1,176)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	10	0.61
(1,153)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	5	0.61
(1,26)	1:3:A:GLU:H	1:3:A:GLU:HG2	9	0.61
(1,26)	1:3:A:GLU:H	1:3:A:GLU:HG3	9	0.61
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	9	0.6
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	9	0.6
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	9	0.6
(3,203)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	8	0.6
(3,39)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	4	0.6
(3,39)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	7	0.6
(3,39)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	8	0.6
(3,39)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	9	0.6
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	9	0.6
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	9	0.6
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	9	0.6
(2,228)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	8	0.6
(2,45)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	4	0.6
(2,45)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	7	0.6
(2,45)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	8	0.6
(2,45)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	9	0.6
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG21	4	0.6
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG22	4	0.6
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG23	4	0.6
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	10	0.6
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	10	0.6
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	10	0.6
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	2	0.6
(1,608)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	2	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	2	0.6
(1,608)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	2	0.6
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	2	0.6
(1,608)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	2	0.6
(1,592)	1:2:A:GLU:HB2	1:6:A:ARG:H	4	0.6
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD21	8	0.6
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD22	8	0.6
(1,571)	1:9:A:ILE:HA	1:12:A:LEU:HD23	8	0.6
(1,467)	1:23:A:PRO:HA	1:23:A:PRO:HB3	5	0.6
(1,433)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	1	0.6
(1,390)	1:13:A:LYS:HA	1:13:A:LYS:HD2	1	0.6
(1,377)	1:12:A:LEU:HA	1:12:A:LEU:HD11	2	0.6
(1,377)	1:12:A:LEU:HA	1:12:A:LEU:HD12	2	0.6
(1,377)	1:12:A:LEU:HA	1:12:A:LEU:HD13	2	0.6
(1,374)	1:12:A:LEU:HA	1:12:A:LEU:HG	8	0.6
(1,294)	1:2:A:GLU:HA	1:2:A:GLU:HB3	2	0.6
(1,199)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	7	0.6
(1,199)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	7	0.6
(1,199)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	7	0.6
(1,176)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	8	0.6
(1,176)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	8	0.6
(1,153)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	3	0.6
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	7	0.6
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	7	0.6
(1,72)	1:25:A:CYS:H	1:25:A:CYS:HB2	3	0.6
(1,64)	1:18:A:SER:H	1:18:A:SER:HB2	5	0.6
(1,63)	1:18:A:SER:H	1:18:A:SER:HB3	8	0.6
(1,63)	1:18:A:SER:H	1:18:A:SER:HB3	9	0.6
(3,39)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	5	0.59
(3,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	8	0.59
(2,45)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	5	0.59
(2,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	8	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	2	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	2	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	3	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	3	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	4	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	4	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	5	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	5	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	9	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	9	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	10	0.59
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	10	0.59
(1,600)	1:11:A:TRP:HZ3	1:17:A:PRO:HD3	5	0.59
(1,580)	1:5:A:VAL:HG11	1:9:A:ILE:H	1	0.59
(1,580)	1:5:A:VAL:HG12	1:9:A:ILE:H	1	0.59
(1,580)	1:5:A:VAL:HG13	1:9:A:ILE:H	1	0.59
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	7	0.59
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	7	0.59
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	7	0.59
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	7	0.59
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	7	0.59
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	7	0.59
(1,446)	1:22:A:PRO:HA	1:22:A:PRO:HG2	10	0.59
(1,442)	1:22:A:PRO:HA	1:22:A:PRO:HD3	5	0.59
(1,403)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	8	0.59
(1,377)	1:12:A:LEU:HA	1:12:A:LEU:HD11	7	0.59
(1,377)	1:12:A:LEU:HA	1:12:A:LEU:HD12	7	0.59
(1,377)	1:12:A:LEU:HA	1:12:A:LEU:HD13	7	0.59
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	10	0.59
(1,246)	1:8:A:TYR:HD1	1:25:A:CYS:H	1	0.59
(1,246)	1:8:A:TYR:HD2	1:25:A:CYS:H	1	0.59
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	9	0.59
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	9	0.59
(1,176)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	9	0.59
(1,176)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	9	0.59
(1,153)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	4	0.59
(1,153)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	7	0.59
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	3	0.58
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	3	0.58
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	3	0.58
(3,69)	1:19:A:SER:H	1:19:A:SER:HB2	2	0.58
(3,69)	1:19:A:SER:H	1:19:A:SER:HB2	7	0.58
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	3	0.58
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	3	0.58
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	3	0.58
(2,76)	1:19:A:SER:H	1:19:A:SER:HB2	2	0.58
(2,76)	1:19:A:SER:H	1:19:A:SER:HB2	7	0.58
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	10	0.58
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	10	0.58
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	10	0.58
(1,623)	1:5:A:VAL:HA	1:25:A:CYS:HB2	7	0.58
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	7	0.58
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	7	0.58
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	7	0.58
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	7	0.58
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	7	0.58
(1,446)	1:22:A:PRO:HA	1:22:A:PRO:HG2	4	0.58
(1,318)	1:6:A:ARG:HA	1:6:A:ARG:HG3	3	0.58
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	8	0.58
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	8	0.58
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	2	0.58
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	2	0.58
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	7	0.58
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	7	0.58
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	7	0.58
(1,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	2	0.58
(1,153)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	6	0.58
(1,9)	1:7:A:LEU:HD11	1:8:A:TYR:H	1	0.58
(1,9)	1:7:A:LEU:HD12	1:8:A:TYR:H	1	0.58
(1,9)	1:7:A:LEU:HD13	1:8:A:TYR:H	1	0.58
(1,9)	1:7:A:LEU:HD21	1:8:A:TYR:H	1	0.58
(1,9)	1:7:A:LEU:HD22	1:8:A:TYR:H	1	0.58
(1,9)	1:7:A:LEU:HD23	1:8:A:TYR:H	1	0.58
(3,594)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	10	0.57
(3,594)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	10	0.57
(3,594)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	10	0.57
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	4	0.57
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	4	0.57
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	4	0.57
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	3	0.57
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	3	0.57
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	3	0.57
(3,203)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	1	0.57
(3,203)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	9	0.57
(3,185)	1:23:A:PRO:HB3	1:25:A:CYS:H	6	0.57
(3,69)	1:19:A:SER:H	1:19:A:SER:HB2	4	0.57
(3,69)	1:19:A:SER:H	1:19:A:SER:HB2	5	0.57
(3,69)	1:19:A:SER:H	1:19:A:SER:HB2	6	0.57
(3,69)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.57
(3,41)	1:2:A:GLU:HG3	1:5:A:VAL:H	4	0.57
(2,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	10	0.57
(2,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	10	0.57
(2,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	4	0.57
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	4	0.57
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	4	0.57
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	3	0.57
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	3	0.57
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	3	0.57
(2,228)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	1	0.57
(2,228)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	9	0.57
(2,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	6	0.57
(2,76)	1:19:A:SER:H	1:19:A:SER:HB2	4	0.57
(2,76)	1:19:A:SER:H	1:19:A:SER:HB2	5	0.57
(2,76)	1:19:A:SER:H	1:19:A:SER:HB2	6	0.57
(2,76)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.57
(2,47)	1:2:A:GLU:HG3	1:5:A:VAL:H	4	0.57
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	2	0.57
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	2	0.57
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	2	0.57
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	2	0.57
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	2	0.57
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	2	0.57
(1,501)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	2	0.57
(1,446)	1:22:A:PRO:HA	1:22:A:PRO:HG2	6	0.57
(1,446)	1:22:A:PRO:HA	1:22:A:PRO:HG2	9	0.57
(1,442)	1:22:A:PRO:HA	1:22:A:PRO:HD3	3	0.57
(1,442)	1:22:A:PRO:HA	1:22:A:PRO:HD3	8	0.57
(1,421)	1:18:A:SER:HA	1:18:A:SER:HB3	5	0.57
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	9	0.57
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	9	0.57
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	9	0.57
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	9	0.57
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	9	0.57
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	9	0.57
(1,324)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	5	0.57
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	1	0.57
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	1	0.57
(1,208)	1:11:A:TRP:HZ2	1:23:A:PRO:HG3	2	0.57
(1,143)	1:23:A:PRO:HB2	1:25:A:CYS:H	9	0.57
(1,72)	1:25:A:CYS:H	1:25:A:CYS:HB2	6	0.57
(1,72)	1:25:A:CYS:H	1:25:A:CYS:HB2	10	0.57
(1,22)	1:13:A:LYS:H	1:13:A:LYS:HD2	6	0.57
(1,9)	1:7:A:LEU:HD11	1:8:A:TYR:H	10	0.57
(1,9)	1:7:A:LEU:HD12	1:8:A:TYR:H	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:7:A:LEU:HD13	1:8:A:TYR:H	10	0.57
(1,9)	1:7:A:LEU:HD21	1:8:A:TYR:H	10	0.57
(1,9)	1:7:A:LEU:HD22	1:8:A:TYR:H	10	0.57
(1,9)	1:7:A:LEU:HD23	1:8:A:TYR:H	10	0.57
(3,594)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	4	0.56
(3,594)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	4	0.56
(3,594)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	4	0.56
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	1	0.56
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	1	0.56
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	1	0.56
(3,501)	1:3:A:GLU:HA	1:6:A:ARG:HB3	5	0.56
(3,245)	1:8:A:TYR:H	1:9:A:ILE:HG12	2	0.56
(3,201)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	7	0.56
(3,166)	1:11:A:TRP:HE3	1:23:A:PRO:HB2	2	0.56
(3,69)	1:19:A:SER:H	1:19:A:SER:HB2	3	0.56
(2,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	4	0.56
(2,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	4	0.56
(2,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	4	0.56
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	1	0.56
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	1	0.56
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	1	0.56
(2,539)	1:3:A:GLU:HA	1:6:A:ARG:HB3	5	0.56
(2,270)	1:8:A:TYR:H	1:9:A:ILE:HG12	2	0.56
(2,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	7	0.56
(2,183)	1:11:A:TRP:HE3	1:23:A:PRO:HB2	2	0.56
(2,76)	1:19:A:SER:H	1:19:A:SER:HB2	3	0.56
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	8	0.56
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	8	0.56
(1,650)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	8	0.56
(1,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	8	0.56
(1,628)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	2	0.56
(1,593)	1:2:A:GLU:HB3	1:6:A:ARG:H	1	0.56
(1,580)	1:5:A:VAL:HG11	1:9:A:ILE:H	9	0.56
(1,580)	1:5:A:VAL:HG12	1:9:A:ILE:H	9	0.56
(1,580)	1:5:A:VAL:HG13	1:9:A:ILE:H	9	0.56
(1,442)	1:22:A:PRO:HA	1:22:A:PRO:HD3	2	0.56
(1,421)	1:18:A:SER:HA	1:18:A:SER:HB3	4	0.56
(1,374)	1:12:A:LEU:HA	1:12:A:LEU:HG	9	0.56
(1,361)	1:10:A:GLN:HA	1:10:A:GLN:HG2	10	0.56
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	1	0.56
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	1	0.56
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	1	0.56
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	1	0.56
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	1	0.56
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	7	0.56
(1,244)	1:8:A:TYR:HD1	1:9:A:ILE:H	7	0.56
(1,244)	1:8:A:TYR:HD2	1:9:A:ILE:H	7	0.56
(1,234)	1:14:A:ASP:HB3	1:15:A:GLY:H	3	0.56
(1,234)	1:14:A:ASP:HB3	1:15:A:GLY:H	5	0.56
(1,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	2	0.56
(1,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	3	0.56
(1,176)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	3	0.56
(1,176)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	3	0.56
(1,143)	1:23:A:PRO:HB2	1:25:A:CYS:H	5	0.56
(1,72)	1:25:A:CYS:H	1:25:A:CYS:HB2	1	0.56
(1,64)	1:18:A:SER:H	1:18:A:SER:HB2	9	0.56
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	4	0.55
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	4	0.55
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	4	0.55
(3,385)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	3	0.55
(3,385)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	4	0.55
(3,385)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	5	0.55
(3,385)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	7	0.55
(3,107)	1:24:A:PRO:HB3	1:25:A:CYS:H	5	0.55
(3,69)	1:19:A:SER:H	1:19:A:SER:HB2	9	0.55
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	4	0.55
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	4	0.55
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	4	0.55
(2,419)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	3	0.55
(2,419)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	4	0.55
(2,419)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	5	0.55
(2,419)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	7	0.55
(2,116)	1:24:A:PRO:HB3	1:25:A:CYS:H	5	0.55
(2,76)	1:19:A:SER:H	1:19:A:SER:HB2	9	0.55
(1,630)	1:2:A:GLU:HG2	1:5:A:VAL:HB	8	0.55
(1,630)	1:2:A:GLU:HG3	1:5:A:VAL:HB	8	0.55
(1,501)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	4	0.55
(1,501)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	5	0.55
(1,501)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	7	0.55
(1,477)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	6	0.55
(1,477)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	9	0.55
(1,477)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.55
(1,446)	1:22:A:PRO:HA	1:22:A:PRO:HG2	5	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:22:A:PRO:HA	1:22:A:PRO:HG2	7	0.55
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG2	1	0.55
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG3	1	0.55
(1,374)	1:12:A:LEU:HA	1:12:A:LEU:HG	10	0.55
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	10	0.55
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	10	0.55
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	10	0.55
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	10	0.55
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	10	0.55
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	10	0.55
(1,294)	1:2:A:GLU:HA	1:2:A:GLU:HB3	10	0.55
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	4	0.55
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	3	0.55
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	3	0.55
(1,63)	1:18:A:SER:H	1:18:A:SER:HB3	1	0.55
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	6	0.54
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	6	0.54
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	6	0.54
(3,385)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	1	0.54
(3,385)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	8	0.54
(3,385)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	9	0.54
(3,385)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	10	0.54
(3,201)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	5	0.54
(3,107)	1:24:A:PRO:HB3	1:25:A:CYS:H	4	0.54
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	6	0.54
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	6	0.54
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	6	0.54
(2,419)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	1	0.54
(2,419)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	8	0.54
(2,419)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	9	0.54
(2,419)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	10	0.54
(2,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	5	0.54
(2,116)	1:24:A:PRO:HB3	1:25:A:CYS:H	4	0.54
(1,664)	1:10:A:GLN:HA	1:13:A:LYS:HD2	10	0.54
(1,630)	1:2:A:GLU:HG2	1:5:A:VAL:HB	2	0.54
(1,630)	1:2:A:GLU:HG3	1:5:A:VAL:HB	2	0.54
(1,588)	1:14:A:ASP:HB3	1:15:A:GLY:H	9	0.54
(1,501)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	3	0.54
(1,501)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	6	0.54
(1,477)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	3	0.54
(1,477)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	7	0.54
(1,477)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:21:A:ARG:HA	1:22:A:PRO:HD3	2	0.54
(1,442)	1:22:A:PRO:HA	1:22:A:PRO:HD3	1	0.54
(1,421)	1:18:A:SER:HA	1:18:A:SER:HB3	7	0.54
(1,322)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	3	0.54
(1,318)	1:6:A:ARG:HA	1:6:A:ARG:HG3	6	0.54
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	6	0.54
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.54
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	10	0.54
(1,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	5	0.54
(1,182)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	6	0.54
(1,182)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	6	0.54
(1,115)	1:2:A:GLU:HB3	1:5:A:VAL:H	8	0.54
(3,594)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	6	0.53
(3,594)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	6	0.53
(3,594)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	6	0.53
(3,594)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	9	0.53
(3,594)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	9	0.53
(3,594)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	9	0.53
(3,385)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	2	0.53
(3,385)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	6	0.53
(3,171)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	5	0.53
(3,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	7	0.53
(2,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	6	0.53
(2,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	6	0.53
(2,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	6	0.53
(2,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	9	0.53
(2,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	9	0.53
(2,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	9	0.53
(2,419)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	2	0.53
(2,419)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	6	0.53
(2,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	5	0.53
(2,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	7	0.53
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	10	0.53
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	10	0.53
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	10	0.53
(1,501)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	1	0.53
(1,501)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	8	0.53
(1,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	9	0.53
(1,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	0.53
(1,477)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	1	0.53
(1,477)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	4	0.53
(1,477)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:22:A:PRO:HA	1:22:A:PRO:HG2	8	0.53
(1,360)	1:10:A:GLN:HA	1:10:A:GLN:HG3	4	0.53
(1,346)	1:9:A:ILE:HA	1:9:A:ILE:HG12	5	0.53
(1,324)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	10	0.53
(1,294)	1:2:A:GLU:HA	1:2:A:GLU:HB3	5	0.53
(1,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	1	0.53
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	3	0.53
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	3	0.53
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	2	0.53
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	2	0.53
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	2	0.53
(1,189)	1:11:A:TRP:HD1	1:16:A:GLY:HA3	4	0.53
(1,182)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	10	0.53
(1,182)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	10	0.53
(1,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	7	0.53
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	10	0.53
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	10	0.53
(1,43)	1:4:A:CYS:HB3	1:5:A:VAL:H	7	0.53
(1,26)	1:3:A:GLU:H	1:3:A:GLU:HG2	6	0.53
(1,26)	1:3:A:GLU:H	1:3:A:GLU:HG3	6	0.53
(3,594)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	1	0.52
(3,594)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	1	0.52
(3,594)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	1	0.52
(3,594)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	8	0.52
(3,594)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	8	0.52
(3,594)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	8	0.52
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	10	0.52
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	10	0.52
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	10	0.52
(3,492)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	1	0.52
(3,185)	1:23:A:PRO:HB3	1:25:A:CYS:H	8	0.52
(3,13)	1:6:A:ARG:H	1:6:A:ARG:HG3	5	0.52
(2,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	1	0.52
(2,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	1	0.52
(2,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	1	0.52
(2,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	8	0.52
(2,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	8	0.52
(2,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	8	0.52
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	10	0.52
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	10	0.52
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	10	0.52
(2,530)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	8	0.52
(2,17)	1:6:A:ARG:H	1:6:A:ARG:HG3	5	0.52
(1,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	5	0.52
(1,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	5	0.52
(1,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	5	0.52
(1,501)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	9	0.52
(1,501)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.52
(1,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	1	0.52
(1,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	3	0.52
(1,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	6	0.52
(1,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	8	0.52
(1,374)	1:12:A:LEU:HA	1:12:A:LEU:HG	1	0.52
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD11	4	0.52
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD12	4	0.52
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD13	4	0.52
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.52
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.52
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.52
(1,326)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	8	0.52
(1,246)	1:8:A:TYR:HD1	1:25:A:CYS:H	10	0.52
(1,246)	1:8:A:TYR:HD2	1:25:A:CYS:H	10	0.52
(1,244)	1:8:A:TYR:HD1	1:9:A:ILE:H	2	0.52
(1,244)	1:8:A:TYR:HD2	1:9:A:ILE:H	2	0.52
(1,176)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	7	0.52
(1,176)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	7	0.52
(1,153)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	2	0.52
(1,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	4	0.52
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG21	3	0.52
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG22	3	0.52
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG23	3	0.52
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	6	0.51
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	6	0.51
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	6	0.51
(3,572)	1:17:A:PRO:HB2	1:18:A:SER:HB2	6	0.51
(3,185)	1:23:A:PRO:HB3	1:25:A:CYS:H	5	0.51
(3,171)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	6	0.51
(3,162)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	9	0.51
(3,107)	1:24:A:PRO:HB3	1:25:A:CYS:H	8	0.51
(3,69)	1:19:A:SER:H	1:19:A:SER:HB2	1	0.51
(3,21)	1:2:A:GLU:HB2	1:3:A:GLU:H	6	0.51
(3,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	2	0.51
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	6	0.51
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	6	0.51
(2,616)	1:17:A:PRO:HB2	1:18:A:SER:HB2	6	0.51
(2,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	5	0.51
(2,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	6	0.51
(2,179)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	9	0.51
(2,116)	1:24:A:PRO:HB3	1:25:A:CYS:H	8	0.51
(2,76)	1:19:A:SER:H	1:19:A:SER:HB2	1	0.51
(2,25)	1:2:A:GLU:HB2	1:3:A:GLU:H	6	0.51
(2,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	2	0.51
(1,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	4	0.51
(1,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	4	0.51
(1,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	4	0.51
(1,634)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	10	0.51
(1,634)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	10	0.51
(1,634)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	10	0.51
(1,630)	1:2:A:GLU:HG2	1:5:A:VAL:HB	10	0.51
(1,630)	1:2:A:GLU:HG3	1:5:A:VAL:HB	10	0.51
(1,629)	1:2:A:GLU:HG3	1:5:A:VAL:HB	7	0.51
(1,597)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	2	0.51
(1,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	4	0.51
(1,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	7	0.51
(1,479)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	5	0.51
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	8	0.51
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	8	0.51
(1,326)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	1	0.51
(1,326)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	6	0.51
(1,323)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	1	0.51
(1,294)	1:2:A:GLU:HA	1:2:A:GLU:HB3	8	0.51
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	2	0.51
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	1	0.51
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	1	0.51
(1,43)	1:4:A:CYS:HB3	1:5:A:VAL:H	6	0.51
(3,594)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	3	0.5
(3,594)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	3	0.5
(3,594)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	3	0.5
(3,203)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	6	0.5
(3,163)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	2	0.5
(3,107)	1:24:A:PRO:HB3	1:25:A:CYS:H	2	0.5
(3,107)	1:24:A:PRO:HB3	1:25:A:CYS:H	7	0.5
(3,107)	1:24:A:PRO:HB3	1:25:A:CYS:H	9	0.5
(2,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	3	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	3	0.5
(2,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	3	0.5
(2,228)	1:11:A:TRP:HZ3	1:17:A:PRO:HG2	6	0.5
(2,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	2	0.5
(2,116)	1:24:A:PRO:HB3	1:25:A:CYS:H	2	0.5
(2,116)	1:24:A:PRO:HB3	1:25:A:CYS:H	7	0.5
(2,116)	1:24:A:PRO:HB3	1:25:A:CYS:H	9	0.5
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	8	0.5
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	8	0.5
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	8	0.5
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG21	10	0.5
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG22	10	0.5
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG23	10	0.5
(1,552)	1:22:A:PRO:HA	1:23:A:PRO:HD3	2	0.5
(1,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	5	0.5
(1,479)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	4	0.5
(1,463)	1:21:A:ARG:HA	1:22:A:PRO:HD3	3	0.5
(1,374)	1:12:A:LEU:HA	1:12:A:LEU:HG	3	0.5
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD11	7	0.5
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD12	7	0.5
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD13	7	0.5
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.5
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.5
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.5
(1,319)	1:6:A:ARG:HA	1:6:A:ARG:HG2	6	0.5
(1,246)	1:8:A:TYR:HD1	1:25:A:CYS:H	3	0.5
(1,246)	1:8:A:TYR:HD2	1:25:A:CYS:H	3	0.5
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	8	0.5
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	8	0.5
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	8	0.5
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	8	0.5
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	8	0.5
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	8	0.5
(1,71)	1:25:A:CYS:H	1:25:A:CYS:HB3	5	0.5
(1,44)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	4	0.5
(1,44)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	5	0.5
(1,22)	1:13:A:LYS:H	1:13:A:LYS:HD2	3	0.5
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	7	0.49
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	7	0.49
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	7	0.49
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	7	0.49
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	7	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	7	0.49
(3,126)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	6	0.49
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	7	0.49
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	7	0.49
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	7	0.49
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	7	0.49
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	7	0.49
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	7	0.49
(2,137)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	6	0.49
(1,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	3	0.49
(1,479)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	1	0.49
(1,463)	1:21:A:ARG:HA	1:22:A:PRO:HD3	1	0.49
(1,462)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	1	0.49
(1,462)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	2	0.49
(1,374)	1:12:A:LEU:HA	1:12:A:LEU:HG	6	0.49
(1,326)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	4	0.49
(1,323)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	8	0.49
(1,268)	1:8:A:TYR:H	1:24:A:PRO:HG2	2	0.49
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	1	0.49
(1,143)	1:23:A:PRO:HB2	1:25:A:CYS:H	8	0.49
(1,75)	1:19:A:SER:H	1:19:A:SER:HB3	1	0.49
(1,44)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	7	0.49
(1,44)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	8	0.49
(1,44)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	9	0.49
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	1	0.48
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	1	0.48
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	1	0.48
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	1	0.48
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	1	0.48
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	1	0.48
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD11	8	0.48
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD12	8	0.48
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD13	8	0.48
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	1	0.48
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	1	0.48
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	1	0.48
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	10	0.48
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	10	0.48
(3,591)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	10	0.48
(3,567)	1:15:A:GLY:HA3	1:18:A:SER:HB3	7	0.48
(3,550)	1:2:A:GLU:HB2	1:5:A:VAL:H	3	0.48
(3,107)	1:24:A:PRO:HB3	1:25:A:CYS:H	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,46)	1:21:A:ARG:H	1:21:A:ARG:HB3	1	0.48
(3,13)	1:6:A:ARG:H	1:6:A:ARG:HG3	1	0.48
(3,13)	1:6:A:ARG:H	1:6:A:ARG:HG3	10	0.48
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	1	0.48
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	1	0.48
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	1	0.48
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	10	0.48
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	10	0.48
(2,636)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	10	0.48
(2,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	7	0.48
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	1	0.48
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	1	0.48
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	1	0.48
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	1	0.48
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	1	0.48
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	1	0.48
(2,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	3	0.48
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD11	8	0.48
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD12	8	0.48
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD13	8	0.48
(2,116)	1:24:A:PRO:HB3	1:25:A:CYS:H	10	0.48
(2,52)	1:21:A:ARG:H	1:21:A:ARG:HB3	1	0.48
(2,17)	1:6:A:ARG:H	1:6:A:ARG:HG3	1	0.48
(2,17)	1:6:A:ARG:H	1:6:A:ARG:HG3	10	0.48
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	8	0.48
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	8	0.48
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	8	0.48
(1,630)	1:2:A:GLU:HG2	1:5:A:VAL:HB	5	0.48
(1,630)	1:2:A:GLU:HG3	1:5:A:VAL:HB	5	0.48
(1,630)	1:2:A:GLU:HG2	1:5:A:VAL:HB	6	0.48
(1,630)	1:2:A:GLU:HG3	1:5:A:VAL:HB	6	0.48
(1,479)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	8	0.48
(1,462)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	3	0.48
(1,462)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	8	0.48
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG2	8	0.48
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG3	8	0.48
(1,374)	1:12:A:LEU:HA	1:12:A:LEU:HG	4	0.48
(1,360)	1:10:A:GLN:HA	1:10:A:GLN:HG3	7	0.48
(1,346)	1:9:A:ILE:HA	1:9:A:ILE:HG12	8	0.48
(1,318)	1:6:A:ARG:HA	1:6:A:ARG:HG3	9	0.48
(1,110)	1:12:A:LEU:H	1:12:A:LEU:HG	5	0.48
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	4	0.47
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	4	0.47
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	4	0.47
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	4	0.47
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	4	0.47
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD11	9	0.47
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD12	9	0.47
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD13	9	0.47
(4,23)	1:11:A:TRP:HE3	1:12:A:LEU:HG	9	0.47
(3,320)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.47
(3,320)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.47
(3,320)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.47
(3,245)	1:8:A:TYR:H	1:9:A:ILE:HG12	5	0.47
(3,201)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	4	0.47
(3,162)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	6	0.47
(3,13)	1:6:A:ARG:H	1:6:A:ARG:HG3	8	0.47
(3,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	10	0.47
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	4	0.47
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	4	0.47
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	4	0.47
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	4	0.47
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	4	0.47
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	4	0.47
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD11	9	0.47
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD12	9	0.47
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD13	9	0.47
(2,351)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.47
(2,351)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.47
(2,351)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.47
(2,270)	1:8:A:TYR:H	1:9:A:ILE:HG12	5	0.47
(2,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	4	0.47
(2,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	9	0.47
(2,179)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	6	0.47
(2,17)	1:6:A:ARG:H	1:6:A:ARG:HG3	8	0.47
(2,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	10	0.47
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG2	9	0.47
(1,667)	1:1:A:GLU:HA	1:1:A:GLU:HG3	9	0.47
(1,661)	1:9:A:ILE:HA	1:12:A:LEU:HB2	2	0.47
(1,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	6	0.47
(1,583)	1:6:A:ARG:HB3	1:7:A:LEU:H	6	0.47
(1,577)	1:20:A:GLY:H	1:21:A:ARG:H	10	0.47
(1,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB2	4	0.47
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB3	4	0.47
(1,538)	1:7:A:LEU:HA	1:10:A:GLN:HB3	6	0.47
(1,531)	1:11:A:TRP:HB3	1:24:A:PRO:HG3	7	0.47
(1,462)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	5	0.47
(1,462)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	7	0.47
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	2	0.47
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	2	0.47
(1,430)	1:21:A:ARG:HA	1:21:A:ARG:HB3	1	0.47
(1,430)	1:21:A:ARG:HA	1:21:A:ARG:HB3	2	0.47
(1,430)	1:21:A:ARG:HA	1:21:A:ARG:HB3	4	0.47
(1,430)	1:21:A:ARG:HA	1:21:A:ARG:HB3	7	0.47
(1,374)	1:12:A:LEU:HA	1:12:A:LEU:HG	5	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD11	8	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD12	8	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD13	8	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	0.47
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	0.47
(1,326)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	7	0.47
(1,326)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	9	0.47
(1,322)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	6	0.47
(1,294)	1:2:A:GLU:HA	1:2:A:GLU:HB3	7	0.47
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	4	0.47
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	4	0.47
(1,222)	1:8:A:TYR:HE1	1:9:A:ILE:HG12	5	0.47
(1,222)	1:8:A:TYR:HE2	1:9:A:ILE:HG12	5	0.47
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	8	0.47
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	8	0.47
(1,44)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	3	0.47
(1,22)	1:13:A:LYS:H	1:13:A:LYS:HD2	7	0.47
(1,22)	1:13:A:LYS:H	1:13:A:LYS:HD2	9	0.47
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD11	1	0.46
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD12	1	0.46
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD13	1	0.46
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD11	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD12	6	0.46
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD13	6	0.46
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	2	0.46
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	2	0.46
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	2	0.46
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	2	0.46
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	2	0.46
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	2	0.46
(3,584)	1:2:A:GLU:HG3	1:5:A:VAL:HB	4	0.46
(3,245)	1:8:A:TYR:H	1:9:A:ILE:HG12	7	0.46
(3,193)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.46
(3,193)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.46
(3,171)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	1	0.46
(3,107)	1:24:A:PRO:HB3	1:25:A:CYS:H	1	0.46
(3,46)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.46
(3,46)	1:21:A:ARG:H	1:21:A:ARG:HB3	8	0.46
(2,629)	1:2:A:GLU:HG3	1:5:A:VAL:HB	4	0.46
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD11	1	0.46
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD12	1	0.46
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD13	1	0.46
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD11	6	0.46
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD12	6	0.46
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD13	6	0.46
(2,270)	1:8:A:TYR:H	1:9:A:ILE:HG12	7	0.46
(2,217)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.46
(2,217)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.46
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	2	0.46
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	2	0.46
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	2	0.46
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	2	0.46
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	2	0.46
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	2	0.46
(2,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	1	0.46
(2,116)	1:24:A:PRO:HB3	1:25:A:CYS:H	1	0.46
(2,52)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.46
(2,52)	1:21:A:ARG:H	1:21:A:ARG:HB3	8	0.46
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	6	0.46
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	6	0.46
(1,656)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	6	0.46
(1,630)	1:2:A:GLU:HG2	1:5:A:VAL:HB	4	0.46
(1,630)	1:2:A:GLU:HG3	1:5:A:VAL:HB	4	0.46
(1,597)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,597)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	8	0.46
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	9	0.46
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	9	0.46
(1,496)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	2	0.46
(1,479)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	7	0.46
(1,462)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	4	0.46
(1,462)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	6	0.46
(1,462)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	9	0.46
(1,462)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	10	0.46
(1,455)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	7	0.46
(1,455)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	8	0.46
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	1	0.46
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	1	0.46
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	3	0.46
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	3	0.46
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	4	0.46
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	4	0.46
(1,430)	1:21:A:ARG:HA	1:21:A:ARG:HB3	3	0.46
(1,430)	1:21:A:ARG:HA	1:21:A:ARG:HB3	6	0.46
(1,430)	1:21:A:ARG:HA	1:21:A:ARG:HB3	9	0.46
(1,430)	1:21:A:ARG:HA	1:21:A:ARG:HB3	10	0.46
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG2	2	0.46
(1,392)	1:13:A:LYS:HA	1:13:A:LYS:HG3	2	0.46
(1,346)	1:9:A:ILE:HA	1:9:A:ILE:HG12	4	0.46
(1,326)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	5	0.46
(1,294)	1:2:A:GLU:HA	1:2:A:GLU:HB3	1	0.46
(1,294)	1:2:A:GLU:HA	1:2:A:GLU:HB3	3	0.46
(1,294)	1:2:A:GLU:HA	1:2:A:GLU:HB3	6	0.46
(1,246)	1:8:A:TYR:HD1	1:25:A:CYS:H	9	0.46
(1,246)	1:8:A:TYR:HD2	1:25:A:CYS:H	9	0.46
(1,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	1	0.46
(1,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	1	0.46
(1,182)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	8	0.46
(1,182)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	8	0.46
(1,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	9	0.46
(1,91)	1:11:A:TRP:HE1	1:19:A:SER:HG	1	0.46
(1,44)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	1	0.46
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD11	3	0.45
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD12	3	0.45
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD13	3	0.45
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD11	4	0.45
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD12	4	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD13	4	0.45
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD11	10	0.45
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD12	10	0.45
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD13	10	0.45
(3,250)	1:5:A:VAL:HG21	1:6:A:ARG:H	7	0.45
(3,250)	1:5:A:VAL:HG22	1:6:A:ARG:H	7	0.45
(3,250)	1:5:A:VAL:HG23	1:6:A:ARG:H	7	0.45
(3,193)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	1	0.45
(3,193)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	1	0.45
(3,185)	1:23:A:PRO:HB3	1:25:A:CYS:H	9	0.45
(3,162)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	7	0.45
(3,126)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	3	0.45
(3,126)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	10	0.45
(3,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	9	0.45
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD11	3	0.45
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD12	3	0.45
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD13	3	0.45
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD11	4	0.45
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD12	4	0.45
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD13	4	0.45
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD11	10	0.45
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD12	10	0.45
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD13	10	0.45
(2,278)	1:5:A:VAL:HG21	1:6:A:ARG:H	7	0.45
(2,278)	1:5:A:VAL:HG22	1:6:A:ARG:H	7	0.45
(2,278)	1:5:A:VAL:HG23	1:6:A:ARG:H	7	0.45
(2,217)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	1	0.45
(2,217)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	1	0.45
(2,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	9	0.45
(2,179)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	7	0.45
(2,137)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	3	0.45
(2,137)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	10	0.45
(2,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	9	0.45
(1,661)	1:9:A:ILE:HA	1:12:A:LEU:HB2	7	0.45
(1,597)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	6	0.45
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	4	0.45
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	4	0.45
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	7	0.45
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	7	0.45
(1,479)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	10	0.45
(1,455)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	4	0.45
(1,455)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	6	0.45
(1,455)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	9	0.45
(1,455)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.45
(1,430)	1:21:A:ARG:HA	1:21:A:ARG:HB3	5	0.45
(1,430)	1:21:A:ARG:HA	1:21:A:ARG:HB3	8	0.45
(1,361)	1:10:A:GLN:HA	1:10:A:GLN:HG2	2	0.45
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.45
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.45
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.45
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.45
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.45
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.45
(1,326)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	2	0.45
(1,234)	1:14:A:ASP:HB3	1:15:A:GLY:H	9	0.45
(1,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	5	0.45
(1,43)	1:4:A:CYS:HB3	1:5:A:VAL:H	2	0.45
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	8	0.44
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	8	0.44
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	8	0.44
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	8	0.44
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	8	0.44
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	8	0.44
(4,43)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.44
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD11	7	0.44
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD12	7	0.44
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD13	7	0.44
(4,30)	1:10:A:GLN:HE22	1:11:A:TRP:H	10	0.44
(4,23)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.44
(4,16)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	6	0.44
(4,16)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	6	0.44
(4,11)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.44
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.44
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.44
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.44
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	8	0.44
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	8	0.44
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	8	0.44
(3,193)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	2	0.44
(3,193)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	2	0.44
(3,162)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	2	0.44
(3,107)	1:24:A:PRO:HB3	1:25:A:CYS:H	6	0.44
(3,46)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,46)	1:21:A:ARG:H	1:21:A:ARG:HB3	4	0.44
(3,46)	1:21:A:ARG:H	1:21:A:ARG:HB3	9	0.44
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	8	0.44
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	8	0.44
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	8	0.44
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	8	0.44
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	8	0.44
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	8	0.44
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	8	0.44
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	8	0.44
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	8	0.44
(2,603)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.44
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD11	7	0.44
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD12	7	0.44
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD13	7	0.44
(2,292)	1:10:A:GLN:HE22	1:11:A:TRP:H	10	0.44
(2,217)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	2	0.44
(2,217)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	2	0.44
(2,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.44
(2,179)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	2	0.44
(2,175)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	6	0.44
(2,175)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	6	0.44
(2,132)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.44
(2,116)	1:24:A:PRO:HB3	1:25:A:CYS:H	6	0.44
(2,52)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.44
(2,52)	1:21:A:ARG:H	1:21:A:ARG:HB3	4	0.44
(2,52)	1:21:A:ARG:H	1:21:A:ARG:HB3	9	0.44
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.44
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.44
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.44
(1,647)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	5	0.44
(1,647)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	5	0.44
(1,647)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	5	0.44
(1,601)	1:8:A:TYR:HD1	1:25:A:CYS:HB3	9	0.44
(1,601)	1:8:A:TYR:HD2	1:25:A:CYS:HB3	9	0.44
(1,599)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	4	0.44
(1,599)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	4	0.44
(1,597)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	4	0.44
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB2	9	0.44
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB3	9	0.44
(1,534)	1:21:A:ARG:HB3	1:22:A:PRO:HD2	8	0.44
(1,479)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	5	0.44
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	5	0.44
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	9	0.44
(1,437)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	9	0.44
(1,435)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	3	0.44
(1,435)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	5	0.44
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG2	1	0.44
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG3	1	0.44
(1,405)	1:17:A:PRO:HA	1:17:A:PRO:HD3	5	0.44
(1,360)	1:10:A:GLN:HA	1:10:A:GLN:HG3	5	0.44
(1,346)	1:9:A:ILE:HA	1:9:A:ILE:HG12	9	0.44
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD11	5	0.44
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD12	5	0.44
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD13	5	0.44
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.44
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.44
(1,337)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.44
(1,326)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	10	0.44
(1,318)	1:6:A:ARG:HA	1:6:A:ARG:HG3	4	0.44
(1,294)	1:2:A:GLU:HA	1:2:A:GLU:HB3	9	0.44
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	9	0.44
(1,28)	1:4:A:CYS:H	1:4:A:CYS:HB2	3	0.44
(1,22)	1:13:A:LYS:H	1:13:A:LYS:HD2	8	0.44
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG21	4	0.44
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG22	4	0.44
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG23	4	0.44
(4,47)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	8	0.43
(4,47)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	8	0.43
(4,47)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	8	0.43
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	10	0.43
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	10	0.43
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	10	0.43
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	10	0.43
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	10	0.43
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	10	0.43
(4,43)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.43
(4,43)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.43
(4,43)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.43
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	9	0.43
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	9	0.43
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	9	0.43
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	9	0.43
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	9	0.43
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.43
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.43
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.43
(3,594)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	5	0.43
(3,594)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	5	0.43
(3,594)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	5	0.43
(3,320)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.43
(3,320)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.43
(3,320)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.43
(3,201)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.43
(3,162)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	3	0.43
(3,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	6	0.43
(2,643)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	5	0.43
(2,643)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	5	0.43
(2,643)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	5	0.43
(2,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	8	0.43
(2,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	8	0.43
(2,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	8	0.43
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	10	0.43
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	10	0.43
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	10	0.43
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	10	0.43
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	10	0.43
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	10	0.43
(2,603)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.43
(2,603)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.43
(2,603)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.43
(2,351)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.43
(2,351)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.43
(2,351)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.43
(2,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.43
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	9	0.43
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	9	0.43
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	9	0.43
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	9	0.43
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	9	0.43
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	9	0.43
(2,179)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	3	0.43
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.43
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.43
(2,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	6	0.43
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	8	0.43
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	8	0.43
(1,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	4	0.43
(1,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	10	0.43
(1,599)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	5	0.43
(1,599)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	5	0.43
(1,597)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	3	0.43
(1,597)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	10	0.43
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	6	0.43
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	6	0.43
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	6	0.43
(1,565)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	6	0.43
(1,565)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	6	0.43
(1,565)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	6	0.43
(1,534)	1:21:A:ARG:HB3	1:22:A:PRO:HD2	9	0.43
(1,531)	1:11:A:TRP:HB3	1:24:A:PRO:HG3	2	0.43
(1,453)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	4	0.43
(1,453)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	5	0.43
(1,453)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	6	0.43
(1,453)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	7	0.43
(1,453)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	8	0.43
(1,453)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	9	0.43
(1,449)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	3	0.43
(1,435)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	1	0.43
(1,435)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	2	0.43
(1,435)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	9	0.43
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG2	5	0.43
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG3	5	0.43
(1,346)	1:9:A:ILE:HA	1:9:A:ILE:HG12	3	0.43
(1,346)	1:9:A:ILE:HA	1:9:A:ILE:HG12	6	0.43
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	6	0.43
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	6	0.43
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	6	0.43
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	6	0.43
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	6	0.43
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	6	0.43
(1,268)	1:8:A:TYR:H	1:24:A:PRO:HG2	4	0.43
(1,222)	1:8:A:TYR:HE1	1:9:A:ILE:HG12	2	0.43
(1,222)	1:8:A:TYR:HE2	1:9:A:ILE:HG12	2	0.43
(1,33)	1:10:A:GLN:H	1:10:A:GLN:HB2	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.42
(4,43)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.42
(4,43)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.42
(4,43)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.42
(4,29)	1:9:A:ILE:HD11	1:10:A:GLN:H	7	0.42
(4,29)	1:9:A:ILE:HD12	1:10:A:GLN:H	7	0.42
(4,29)	1:9:A:ILE:HD13	1:10:A:GLN:H	7	0.42
(4,29)	1:9:A:ILE:HD11	1:10:A:GLN:H	8	0.42
(4,29)	1:9:A:ILE:HD12	1:10:A:GLN:H	8	0.42
(4,29)	1:9:A:ILE:HD13	1:10:A:GLN:H	8	0.42
(4,11)	1:12:A:LEU:H	1:13:A:LYS:HA	1	0.42
(4,11)	1:12:A:LEU:H	1:13:A:LYS:HA	4	0.42
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.42
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.42
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.42
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	9	0.42
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	9	0.42
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	9	0.42
(3,320)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.42
(3,193)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	3	0.42
(3,193)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	3	0.42
(3,171)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	3	0.42
(3,171)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	8	0.42
(3,171)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	10	0.42
(3,164)	1:11:A:TRP:HZ3	1:23:A:PRO:HB2	2	0.42
(3,162)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	8	0.42
(3,107)	1:24:A:PRO:HB3	1:25:A:CYS:H	3	0.42
(3,98)	1:6:A:ARG:HG3	1:7:A:LEU:H	7	0.42
(3,46)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.42
(3,32)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.42
(3,13)	1:6:A:ARG:H	1:6:A:ARG:HG3	2	0.42
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	9	0.42
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	9	0.42
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	9	0.42
(2,603)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.42
(2,603)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.42
(2,603)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.42
(2,603)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.42
(2,351)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.42
(2,280)	1:9:A:ILE:HD11	1:10:A:GLN:H	7	0.42
(2,280)	1:9:A:ILE:HD12	1:10:A:GLN:H	7	0.42
(2,280)	1:9:A:ILE:HD13	1:10:A:GLN:H	7	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,280)	1:9:A:ILE:HD11	1:10:A:GLN:H	8	0.42
(2,280)	1:9:A:ILE:HD12	1:10:A:GLN:H	8	0.42
(2,280)	1:9:A:ILE:HD13	1:10:A:GLN:H	8	0.42
(2,217)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	3	0.42
(2,217)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	3	0.42
(2,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	3	0.42
(2,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	8	0.42
(2,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	10	0.42
(2,181)	1:11:A:TRP:HZ3	1:23:A:PRO:HB2	2	0.42
(2,179)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	8	0.42
(2,132)	1:12:A:LEU:H	1:13:A:LYS:HA	1	0.42
(2,132)	1:12:A:LEU:H	1:13:A:LYS:HA	4	0.42
(2,116)	1:24:A:PRO:HB3	1:25:A:CYS:H	3	0.42
(2,106)	1:6:A:ARG:HG3	1:7:A:LEU:H	7	0.42
(2,52)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.42
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.42
(2,17)	1:6:A:ARG:H	1:6:A:ARG:HG3	2	0.42
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.42
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.42
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.42
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	1	0.42
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	1	0.42
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	1	0.42
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	1	0.42
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	1	0.42
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	8	0.42
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	8	0.42
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	8	0.42
(1,647)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	7	0.42
(1,647)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	7	0.42
(1,647)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	7	0.42
(1,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	1	0.42
(1,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	1	0.42
(1,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	1	0.42
(1,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	3	0.42
(1,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	3	0.42
(1,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	3	0.42
(1,629)	1:2:A:GLU:HG3	1:5:A:VAL:HB	3	0.42
(1,564)	1:11:A:TRP:HA	1:14:A:ASP:HB2	6	0.42
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	5	0.42
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	5	0.42
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	5	0.42
(1,561)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	5	0.42
(1,561)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	5	0.42
(1,479)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	6	0.42
(1,479)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	9	0.42
(1,453)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.42
(1,435)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	4	0.42
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG2	6	0.42
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG3	6	0.42
(1,390)	1:13:A:LYS:HA	1:13:A:LYS:HD2	5	0.42
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	1	0.42
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	1	0.42
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	1	0.42
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	8	0.42
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	8	0.42
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	8	0.42
(1,336)	1:7:A:LEU:HA	1:7:A:LEU:HB3	6	0.42
(1,322)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	9	0.42
(1,182)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	9	0.42
(1,182)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	9	0.42
(1,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	0.42
(1,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.42
(4,43)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.41
(4,43)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.41
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	5	0.41
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	5	0.41
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	5	0.41
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	5	0.41
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	5	0.41
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	5	0.41
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	8	0.41
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	8	0.41
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	8	0.41
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	8	0.41
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	8	0.41
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	8	0.41
(4,16)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	1	0.41
(4,16)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	1	0.41
(4,11)	1:12:A:LEU:H	1:13:A:LYS:HA	6	0.41
(3,337)	1:9:A:ILE:HG12	1:10:A:GLN:H	2	0.41
(3,320)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.41
(3,320)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,320)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.41
(3,201)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	3	0.41
(3,193)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	6	0.41
(3,193)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	6	0.41
(3,193)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	9	0.41
(3,193)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	9	0.41
(3,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	1	0.41
(2,603)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.41
(2,603)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.41
(2,369)	1:9:A:ILE:HG12	1:10:A:GLN:H	2	0.41
(2,351)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.41
(2,351)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.41
(2,351)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.41
(2,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	3	0.41
(2,217)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	6	0.41
(2,217)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	6	0.41
(2,217)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	9	0.41
(2,217)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	9	0.41
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	5	0.41
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	5	0.41
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	5	0.41
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	5	0.41
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	5	0.41
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	5	0.41
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	8	0.41
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	8	0.41
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	8	0.41
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	8	0.41
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	8	0.41
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	8	0.41
(2,175)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	1	0.41
(2,175)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	1	0.41
(2,132)	1:12:A:LEU:H	1:13:A:LYS:HA	6	0.41
(2,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	1	0.41
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	6	0.41
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	6	0.41
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	9	0.41
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	9	0.41
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	9	0.41
(1,593)	1:2:A:GLU:HB3	1:6:A:ARG:H	8	0.41
(1,563)	1:18:A:SER:HB3	1:19:A:SER:H	8	0.41
(1,455)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:22:A:PRO:HA	1:22:A:PRO:HG2	3	0.41
(1,405)	1:17:A:PRO:HA	1:17:A:PRO:HD3	7	0.41
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	9	0.41
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	9	0.41
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	9	0.41
(1,346)	1:9:A:ILE:HA	1:9:A:ILE:HG12	10	0.41
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	9	0.41
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	9	0.41
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	9	0.41
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	9	0.41
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	9	0.41
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	9	0.41
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	5	0.41
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	5	0.41
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	7	0.41
(1,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	7	0.41
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	9	0.41
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	9	0.41
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	9	0.41
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	9	0.41
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	9	0.41
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	9	0.41
(1,182)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	3	0.41
(1,182)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	3	0.41
(1,182)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	4	0.41
(1,182)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	4	0.41
(1,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	0.41
(1,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.41
(1,143)	1:23:A:PRO:HB2	1:25:A:CYS:H	6	0.41
(1,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	8	0.41
(1,110)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.41
(1,72)	1:25:A:CYS:H	1:25:A:CYS:HB2	2	0.41
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	1	0.4
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	1	0.4
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	1	0.4
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	1	0.4
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	1	0.4
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	1	0.4
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	1	0.4
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	1	0.4
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	1	0.4
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	6	0.4
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	6	0.4
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	6	0.4
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	6	0.4
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	6	0.4
(4,29)	1:9:A:ILE:HD11	1:10:A:GLN:H	2	0.4
(4,29)	1:9:A:ILE:HD12	1:10:A:GLN:H	2	0.4
(4,29)	1:9:A:ILE:HD13	1:10:A:GLN:H	2	0.4
(4,29)	1:9:A:ILE:HD11	1:10:A:GLN:H	5	0.4
(4,29)	1:9:A:ILE:HD12	1:10:A:GLN:H	5	0.4
(4,29)	1:9:A:ILE:HD13	1:10:A:GLN:H	5	0.4
(4,29)	1:9:A:ILE:HD11	1:10:A:GLN:H	9	0.4
(4,29)	1:9:A:ILE:HD12	1:10:A:GLN:H	9	0.4
(4,29)	1:9:A:ILE:HD13	1:10:A:GLN:H	9	0.4
(4,21)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	2	0.4
(4,21)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	2	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	1	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	1	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	1	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	1	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	1	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	1	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	6	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	6	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	6	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	6	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	6	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	6	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	0.4
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	0.4
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	0.4
(4,17)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	9	0.4
(4,17)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.4
(4,16)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	3	0.4
(4,16)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	3	0.4
(4,16)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	5	0.4
(4,16)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	5	0.4
(4,16)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.4
(4,16)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,480)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	1	0.4
(3,337)	1:9:A:ILE:HG12	1:10:A:GLN:H	5	0.4
(3,250)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	0.4
(3,250)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	0.4
(3,250)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	0.4
(3,189)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	6	0.4
(3,162)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	4	0.4
(3,46)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.4
(3,37)	1:4:A:CYS:HB3	1:5:A:VAL:H	5	0.4
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	1	0.4
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	1	0.4
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	1	0.4
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	1	0.4
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	1	0.4
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	1	0.4
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	1	0.4
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	1	0.4
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	1	0.4
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	6	0.4
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	6	0.4
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	6	0.4
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	6	0.4
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	6	0.4
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	6	0.4
(2,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	1	0.4
(2,369)	1:9:A:ILE:HG12	1:10:A:GLN:H	5	0.4
(2,280)	1:9:A:ILE:HD11	1:10:A:GLN:H	2	0.4
(2,280)	1:9:A:ILE:HD12	1:10:A:GLN:H	2	0.4
(2,280)	1:9:A:ILE:HD13	1:10:A:GLN:H	2	0.4
(2,280)	1:9:A:ILE:HD11	1:10:A:GLN:H	5	0.4
(2,280)	1:9:A:ILE:HD12	1:10:A:GLN:H	5	0.4
(2,280)	1:9:A:ILE:HD13	1:10:A:GLN:H	5	0.4
(2,280)	1:9:A:ILE:HD11	1:10:A:GLN:H	9	0.4
(2,280)	1:9:A:ILE:HD12	1:10:A:GLN:H	9	0.4
(2,280)	1:9:A:ILE:HD13	1:10:A:GLN:H	9	0.4
(2,278)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	0.4
(2,278)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	0.4
(2,278)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	0.4
(2,211)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	6	0.4
(2,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	2	0.4
(2,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	2	0.4
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	1	0.4
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	1	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	1	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	1	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	1	0.4
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	6	0.4
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	6	0.4
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	6	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	6	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	6	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	6	0.4
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	0.4
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	0.4
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	0.4
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	0.4
(2,179)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	4	0.4
(2,177)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	9	0.4
(2,177)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.4
(2,175)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	3	0.4
(2,175)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	3	0.4
(2,175)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	5	0.4
(2,175)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	5	0.4
(2,175)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.4
(2,175)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.4
(2,52)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.4
(2,43)	1:4:A:CYS:HB3	1:5:A:VAL:H	5	0.4
(1,647)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	2	0.4
(1,647)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	2	0.4
(1,647)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	2	0.4
(1,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	3	0.4
(1,600)	1:11:A:TRP:HZ3	1:17:A:PRO:HD3	7	0.4
(1,599)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	2	0.4
(1,599)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	2	0.4
(1,597)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	5	0.4
(1,593)	1:2:A:GLU:HB3	1:6:A:ARG:H	7	0.4
(1,593)	1:2:A:GLU:HB3	1:6:A:ARG:H	9	0.4
(1,531)	1:11:A:TRP:HB3	1:24:A:PRO:HG3	3	0.4
(1,455)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	2	0.4
(1,455)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	3	0.4
(1,453)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:22:A:PRO:HA	1:22:A:PRO:HG2	2	0.4
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG2	2	0.4
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG3	2	0.4
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG2	3	0.4
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG3	3	0.4
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG2	9	0.4
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG3	9	0.4
(1,405)	1:17:A:PRO:HA	1:17:A:PRO:HD3	10	0.4
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	10	0.4
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	10	0.4
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	10	0.4
(1,346)	1:9:A:ILE:HA	1:9:A:ILE:HG12	1	0.4
(1,222)	1:8:A:TYR:HE1	1:9:A:ILE:HG12	7	0.4
(1,222)	1:8:A:TYR:HE2	1:9:A:ILE:HG12	7	0.4
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	3	0.4
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	3	0.4
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	3	0.4
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	3	0.4
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	3	0.4
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	3	0.4
(1,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	0.4
(1,110)	1:12:A:LEU:H	1:12:A:LEU:HG	3	0.4
(1,110)	1:12:A:LEU:H	1:12:A:LEU:HG	6	0.4
(1,50)	1:21:A:ARG:H	1:21:A:ARG:HD3	10	0.4
(1,10)	1:9:A:ILE:H	1:12:A:LEU:HD21	2	0.4
(1,10)	1:9:A:ILE:H	1:12:A:LEU:HD22	2	0.4
(1,10)	1:9:A:ILE:H	1:12:A:LEU:HD23	2	0.4
(4,29)	1:9:A:ILE:HD11	1:10:A:GLN:H	4	0.39
(4,29)	1:9:A:ILE:HD12	1:10:A:GLN:H	4	0.39
(4,29)	1:9:A:ILE:HD13	1:10:A:GLN:H	4	0.39
(4,16)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	0.39
(4,16)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	0.39
(4,11)	1:12:A:LEU:H	1:13:A:LYS:HA	3	0.39
(4,11)	1:12:A:LEU:H	1:13:A:LYS:HA	5	0.39
(4,11)	1:12:A:LEU:H	1:13:A:LYS:HA	9	0.39
(3,567)	1:15:A:GLY:HA3	1:18:A:SER:HB3	5	0.39
(3,480)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	10	0.39
(3,205)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	1	0.39
(3,205)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	3	0.39
(3,205)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	4	0.39
(3,205)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	5	0.39
(3,205)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,205)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	8	0.39
(3,205)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	9	0.39
(3,189)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.39
(3,126)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	5	0.39
(3,32)	1:6:A:ARG:H	1:6:A:ARG:HB3	1	0.39
(2,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	5	0.39
(2,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	10	0.39
(2,280)	1:9:A:ILE:HD11	1:10:A:GLN:H	4	0.39
(2,280)	1:9:A:ILE:HD12	1:10:A:GLN:H	4	0.39
(2,280)	1:9:A:ILE:HD13	1:10:A:GLN:H	4	0.39
(2,230)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	1	0.39
(2,230)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	3	0.39
(2,230)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	4	0.39
(2,230)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	5	0.39
(2,230)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	7	0.39
(2,230)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	8	0.39
(2,230)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	9	0.39
(2,211)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.39
(2,175)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	0.39
(2,175)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	0.39
(2,137)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	5	0.39
(2,132)	1:12:A:LEU:H	1:13:A:LYS:HA	3	0.39
(2,132)	1:12:A:LEU:H	1:13:A:LYS:HA	5	0.39
(2,132)	1:12:A:LEU:H	1:13:A:LYS:HA	9	0.39
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HB3	1	0.39
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	7	0.39
(1,671)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	7	0.39
(1,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	7	0.39
(1,599)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	6	0.39
(1,599)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	6	0.39
(1,592)	1:2:A:GLU:HB2	1:6:A:ARG:H	3	0.39
(1,583)	1:6:A:ARG:HB3	1:7:A:LEU:H	5	0.39
(1,583)	1:6:A:ARG:HB3	1:7:A:LEU:H	9	0.39
(1,534)	1:21:A:ARG:HB3	1:22:A:PRO:HD2	4	0.39
(1,534)	1:21:A:ARG:HB3	1:22:A:PRO:HD2	5	0.39
(1,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	7	0.39
(1,453)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	2	0.39
(1,453)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	3	0.39
(1,449)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	2	0.39
(1,446)	1:22:A:PRO:HA	1:22:A:PRO:HG2	1	0.39
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG2	4	0.39
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG3	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG2	10	0.39
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG3	10	0.39
(1,405)	1:17:A:PRO:HA	1:17:A:PRO:HD3	3	0.39
(1,405)	1:17:A:PRO:HA	1:17:A:PRO:HD3	4	0.39
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	3	0.39
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	3	0.39
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	3	0.39
(1,326)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	3	0.39
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	9	0.39
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	9	0.39
(1,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	4	0.39
(1,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	4	0.39
(1,182)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	5	0.39
(1,182)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	5	0.39
(1,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	0.39
(1,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	0.39
(1,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	0.39
(1,65)	1:18:A:SER:H	1:18:A:SER:HA	8	0.39
(1,50)	1:21:A:ARG:H	1:21:A:ARG:HD3	7	0.39
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG21	6	0.39
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG22	6	0.39
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG23	6	0.39
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	9	0.38
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	9	0.38
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	9	0.38
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	9	0.38
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	9	0.38
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	9	0.38
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD11	2	0.38
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD12	2	0.38
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD13	2	0.38
(4,21)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	7	0.38
(4,21)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	7	0.38
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	4	0.38
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	4	0.38
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	4	0.38
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	4	0.38
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	4	0.38
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	4	0.38
(4,17)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	8	0.38
(4,16)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	4	0.38
(4,16)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,16)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	8	0.38
(4,16)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	8	0.38
(4,11)	1:12:A:LEU:H	1:13:A:LYS:HA	7	0.38
(4,11)	1:12:A:LEU:H	1:13:A:LYS:HA	8	0.38
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.38
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.38
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.38
(3,550)	1:2:A:GLU:HB2	1:5:A:VAL:H	4	0.38
(3,480)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	9	0.38
(3,337)	1:9:A:ILE:HG12	1:10:A:GLN:H	7	0.38
(3,201)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	8	0.38
(3,193)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	4	0.38
(3,193)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	4	0.38
(3,193)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	5	0.38
(3,193)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	5	0.38
(3,189)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	3	0.38
(3,189)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	7	0.38
(3,171)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	4	0.38
(3,126)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	7	0.38
(3,126)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	8	0.38
(3,100)	1:6:A:ARG:HB2	1:7:A:LEU:H	9	0.38
(3,46)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.38
(3,46)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.38
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	9	0.38
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	9	0.38
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	9	0.38
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	9	0.38
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	9	0.38
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	9	0.38
(2,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	4	0.38
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD11	2	0.38
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD12	2	0.38
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD13	2	0.38
(2,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	9	0.38
(2,369)	1:9:A:ILE:HG12	1:10:A:GLN:H	7	0.38
(2,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	8	0.38
(2,217)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	4	0.38
(2,217)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	4	0.38
(2,217)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	5	0.38
(2,217)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	5	0.38
(2,211)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	3	0.38
(2,211)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	7	0.38
(2,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	7	0.38
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	4	0.38
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	4	0.38
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	4	0.38
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	4	0.38
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	4	0.38
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	4	0.38
(2,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	4	0.38
(2,177)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	8	0.38
(2,175)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	4	0.38
(2,175)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	4	0.38
(2,175)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	8	0.38
(2,175)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	8	0.38
(2,137)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	7	0.38
(2,137)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	8	0.38
(2,132)	1:12:A:LEU:H	1:13:A:LYS:HA	7	0.38
(2,132)	1:12:A:LEU:H	1:13:A:LYS:HA	8	0.38
(2,108)	1:6:A:ARG:HB2	1:7:A:LEU:H	9	0.38
(2,52)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.38
(2,52)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.38
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.38
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.38
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.38
(1,662)	1:6:A:ARG:HA	1:9:A:ILE:HG12	2	0.38
(1,634)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	8	0.38
(1,634)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	8	0.38
(1,634)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	8	0.38
(1,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	2	0.38
(1,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	3	0.38
(1,529)	1:11:A:TRP:HB3	1:24:A:PRO:HD2	8	0.38
(1,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	2	0.38
(1,463)	1:21:A:ARG:HA	1:22:A:PRO:HD3	7	0.38
(1,405)	1:17:A:PRO:HA	1:17:A:PRO:HD3	9	0.38
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	6	0.38
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	6	0.38
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	6	0.38
(1,336)	1:7:A:LEU:HA	1:7:A:LEU:HB3	9	0.38
(1,334)	1:7:A:LEU:HA	1:7:A:LEU:HB2	1	0.38
(1,334)	1:7:A:LEU:HA	1:7:A:LEU:HB2	10	0.38
(1,268)	1:8:A:TYR:H	1:24:A:PRO:HG2	3	0.38
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	2	0.38
(1,205)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	2	0.38
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	1	0.38
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	1	0.38
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	1	0.38
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	1	0.38
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	1	0.38
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	1	0.38
(1,143)	1:23:A:PRO:HB2	1:25:A:CYS:H	2	0.38
(1,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	7	0.38
(1,110)	1:12:A:LEU:H	1:12:A:LEU:HG	4	0.38
(1,91)	1:11:A:TRP:HE1	1:19:A:SER:HG	8	0.38
(1,33)	1:10:A:GLN:H	1:10:A:GLN:HB2	4	0.38
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG21	8	0.38
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG22	8	0.38
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG23	8	0.38
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	10	0.37
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	10	0.37
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	10	0.37
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	10	0.37
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	10	0.37
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	10	0.37
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	10	0.37
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	10	0.37
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	10	0.37
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	3	0.37
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	3	0.37
(4,19)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	3	0.37
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	3	0.37
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	3	0.37
(4,19)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	3	0.37
(4,17)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	6	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.37
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.37
(3,201)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	9	0.37
(3,193)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	7	0.37
(3,193)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	7	0.37
(3,193)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	8	0.37
(3,193)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	8	0.37
(3,185)	1:23:A:PRO:HB3	1:25:A:CYS:H	7	0.37
(3,162)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.37
(3,126)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	9	0.37
(3,100)	1:6:A:ARG:HB2	1:7:A:LEU:H	4	0.37
(3,100)	1:6:A:ARG:HB2	1:7:A:LEU:H	6	0.37
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	10	0.37
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	10	0.37
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	10	0.37
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	10	0.37
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	10	0.37
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	10	0.37
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	10	0.37
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	10	0.37
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	10	0.37
(2,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	9	0.37
(2,217)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	7	0.37
(2,217)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	7	0.37
(2,217)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	8	0.37
(2,217)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	8	0.37
(2,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	7	0.37
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	3	0.37
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	3	0.37
(2,195)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	3	0.37
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	3	0.37
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	3	0.37
(2,195)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	3	0.37
(2,179)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.37
(2,177)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	6	0.37
(2,137)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,108)	1:6:A:ARG:HB2	1:7:A:LEU:H	4	0.37
(2,108)	1:6:A:ARG:HB2	1:7:A:LEU:H	6	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.37
(2,5)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.37
(1,657)	1:2:A:GLU:HG2	1:5:A:VAL:HG11	4	0.37
(1,657)	1:2:A:GLU:HG2	1:5:A:VAL:HG12	4	0.37
(1,657)	1:2:A:GLU:HG2	1:5:A:VAL:HG13	4	0.37
(1,634)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	5	0.37
(1,634)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	5	0.37
(1,634)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	5	0.37
(1,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	8	0.37
(1,583)	1:6:A:ARG:HB3	1:7:A:LEU:H	4	0.37
(1,577)	1:20:A:GLY:H	1:21:A:ARG:H	7	0.37
(1,541)	1:4:A:CYS:HA	1:7:A:LEU:HB2	9	0.37
(1,538)	1:7:A:LEU:HA	1:10:A:GLN:HB3	3	0.37
(1,528)	1:11:A:TRP:HB3	1:24:A:PRO:HD3	9	0.37
(1,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	5	0.37
(1,458)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	1	0.37
(1,458)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	2	0.37
(1,458)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	3	0.37
(1,458)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	4	0.37
(1,458)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	5	0.37
(1,458)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	6	0.37
(1,458)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	7	0.37
(1,458)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	8	0.37
(1,458)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.37
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG2	7	0.37
(1,431)	1:21:A:ARG:HA	1:21:A:ARG:HG3	7	0.37
(1,426)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	1	0.37
(1,426)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	3	0.37
(1,426)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	8	0.37
(1,426)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	10	0.37
(1,418)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	6	0.37
(1,405)	1:17:A:PRO:HA	1:17:A:PRO:HD3	8	0.37
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	4	0.37
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	4	0.37
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	4	0.37
(1,380)	1:12:A:LEU:HB3	1:12:A:LEU:HG	5	0.37
(1,334)	1:7:A:LEU:HA	1:7:A:LEU:HB2	9	0.37
(1,322)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	4	0.37
(1,307)	1:4:A:CYS:HA	1:4:A:CYS:HB3	5	0.37
(1,268)	1:8:A:TYR:H	1:24:A:PRO:HG2	8	0.37
(1,205)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	6	0.37
(1,205)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	6	0.37
(1,205)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	8	0.37
(1,205)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	8	0.37
(1,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	0.37
(1,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	0.37
(1,159)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	0.37
(1,110)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.37
(1,72)	1:25:A:CYS:H	1:25:A:CYS:HB2	4	0.37
(1,71)	1:25:A:CYS:H	1:25:A:CYS:HB3	4	0.37
(1,71)	1:25:A:CYS:H	1:25:A:CYS:HB3	8	0.37
(1,71)	1:25:A:CYS:H	1:25:A:CYS:HB3	10	0.37
(1,43)	1:4:A:CYS:HB3	1:5:A:VAL:H	4	0.37
(1,43)	1:4:A:CYS:HB3	1:5:A:VAL:H	8	0.37
(1,33)	1:10:A:GLN:H	1:10:A:GLN:HB2	7	0.37
(1,10)	1:9:A:ILE:H	1:12:A:LEU:HD21	7	0.37
(1,10)	1:9:A:ILE:H	1:12:A:LEU:HD22	7	0.37
(1,10)	1:9:A:ILE:H	1:12:A:LEU:HD23	7	0.37
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG21	9	0.37
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG22	9	0.37
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG23	9	0.37
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.37
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.37
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.37
(4,29)	1:9:A:ILE:HD11	1:10:A:GLN:H	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,29)	1:9:A:ILE:HD12	1:10:A:GLN:H	6	0.36
(4,29)	1:9:A:ILE:HD13	1:10:A:GLN:H	6	0.36
(4,29)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.36
(4,29)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.36
(4,29)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.36
(4,17)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	1	0.36
(4,17)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	5	0.36
(3,501)	1:3:A:GLU:HA	1:6:A:ARG:HB3	3	0.36
(3,480)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	6	0.36
(3,361)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	2	0.36
(3,162)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	1	0.36
(3,100)	1:6:A:ARG:HB2	1:7:A:LEU:H	1	0.36
(3,100)	1:6:A:ARG:HB2	1:7:A:LEU:H	3	0.36
(3,100)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.36
(3,32)	1:6:A:ARG:H	1:6:A:ARG:HB3	2	0.36
(3,32)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.36
(3,26)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.36
(3,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	3	0.36
(3,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	4	0.36
(2,539)	1:3:A:GLU:HA	1:6:A:ARG:HB3	3	0.36
(2,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	6	0.36
(2,394)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	2	0.36
(2,280)	1:9:A:ILE:HD11	1:10:A:GLN:H	6	0.36
(2,280)	1:9:A:ILE:HD12	1:10:A:GLN:H	6	0.36
(2,280)	1:9:A:ILE:HD13	1:10:A:GLN:H	6	0.36
(2,280)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.36
(2,280)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.36
(2,280)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.36
(2,179)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	1	0.36
(2,177)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	1	0.36
(2,177)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	5	0.36
(2,108)	1:6:A:ARG:HB2	1:7:A:LEU:H	1	0.36
(2,108)	1:6:A:ARG:HB2	1:7:A:LEU:H	3	0.36
(2,108)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.36
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HB3	2	0.36
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.36
(2,30)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.36
(2,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	3	0.36
(2,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	4	0.36
(1,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	6	0.36
(1,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	6	0.36
(1,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,600)	1:11:A:TRP:HZ3	1:17:A:PRO:HD3	2	0.36
(1,558)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	5	0.36
(1,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	4	0.36
(1,529)	1:11:A:TRP:HB3	1:24:A:PRO:HD2	6	0.36
(1,529)	1:11:A:TRP:HB3	1:24:A:PRO:HD2	10	0.36
(1,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	3	0.36
(1,488)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	2	0.36
(1,476)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	2	0.36
(1,426)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	2	0.36
(1,426)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	4	0.36
(1,426)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	5	0.36
(1,426)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	6	0.36
(1,426)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	7	0.36
(1,426)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	9	0.36
(1,418)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	1	0.36
(1,418)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	2	0.36
(1,418)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	3	0.36
(1,418)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	4	0.36
(1,418)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	5	0.36
(1,418)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	7	0.36
(1,418)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	8	0.36
(1,418)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	9	0.36
(1,418)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.36
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	6	0.36
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	6	0.36
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	8	0.36
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	8	0.36
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	10	0.36
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	10	0.36
(1,339)	1:7:A:LEU:HD11	1:7:A:LEU:HG	1	0.36
(1,339)	1:7:A:LEU:HD12	1:7:A:LEU:HG	1	0.36
(1,339)	1:7:A:LEU:HD13	1:7:A:LEU:HG	1	0.36
(1,339)	1:7:A:LEU:HD21	1:7:A:LEU:HG	1	0.36
(1,339)	1:7:A:LEU:HD22	1:7:A:LEU:HG	1	0.36
(1,339)	1:7:A:LEU:HD23	1:7:A:LEU:HG	1	0.36
(1,339)	1:7:A:LEU:HD11	1:7:A:LEU:HG	10	0.36
(1,339)	1:7:A:LEU:HD12	1:7:A:LEU:HG	10	0.36
(1,339)	1:7:A:LEU:HD13	1:7:A:LEU:HG	10	0.36
(1,339)	1:7:A:LEU:HD21	1:7:A:LEU:HG	10	0.36
(1,339)	1:7:A:LEU:HD22	1:7:A:LEU:HG	10	0.36
(1,339)	1:7:A:LEU:HD23	1:7:A:LEU:HG	10	0.36
(1,328)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	4	0.36
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	4	0.36
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	4	0.36
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	4	0.36
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	4	0.36
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	4	0.36
(1,134)	1:19:A:SER:HB2	1:21:A:ARG:H	8	0.36
(1,72)	1:25:A:CYS:H	1:25:A:CYS:HB2	8	0.36
(1,65)	1:18:A:SER:H	1:18:A:SER:HA	1	0.36
(1,63)	1:18:A:SER:H	1:18:A:SER:HB3	2	0.36
(1,50)	1:21:A:ARG:H	1:21:A:ARG:HD3	6	0.36
(1,33)	1:10:A:GLN:H	1:10:A:GLN:HB2	5	0.36
(4,16)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	7	0.35
(4,16)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	7	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.35
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.35
(3,250)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	0.35
(3,250)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	0.35
(3,250)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	0.35
(3,162)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	5	0.35
(3,100)	1:6:A:ARG:HB2	1:7:A:LEU:H	5	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.35
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.35
(2,278)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	0.35
(2,278)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	0.35
(2,278)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	0.35
(2,179)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	5	0.35
(2,175)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	7	0.35
(2,175)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	7	0.35
(2,108)	1:6:A:ARG:HB2	1:7:A:LEU:H	5	0.35
(1,640)	1:12:A:LEU:HD21	1:16:A:GLY:HA3	10	0.35
(1,640)	1:12:A:LEU:HD22	1:16:A:GLY:HA3	10	0.35
(1,640)	1:12:A:LEU:HD23	1:16:A:GLY:HA3	10	0.35
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB2	10	0.35
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB3	10	0.35
(1,488)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	1	0.35
(1,488)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	3	0.35
(1,488)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	4	0.35
(1,488)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	5	0.35
(1,488)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	6	0.35
(1,488)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	7	0.35
(1,488)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	8	0.35
(1,488)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	9	0.35
(1,488)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.35
(1,449)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	1	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	1	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	1	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	2	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	2	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	3	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	3	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	4	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	4	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	5	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	5	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	7	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	7	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	9	0.35
(1,413)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	9	0.35
(1,390)	1:13:A:LYS:HA	1:13:A:LYS:HD2	8	0.35
(1,380)	1:12:A:LEU:HB3	1:12:A:LEU:HG	3	0.35
(1,380)	1:12:A:LEU:HB3	1:12:A:LEU:HG	4	0.35
(1,380)	1:12:A:LEU:HB3	1:12:A:LEU:HG	6	0.35
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG21	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG22	3	0.35
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG23	3	0.35
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG21	8	0.35
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG22	8	0.35
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG23	8	0.35
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG21	10	0.35
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG22	10	0.35
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG23	10	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	1	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	1	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	1	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	10	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	10	0.35
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	10	0.35
(1,339)	1:7:A:LEU:HD11	1:7:A:LEU:HG	2	0.35
(1,339)	1:7:A:LEU:HD12	1:7:A:LEU:HG	2	0.35
(1,339)	1:7:A:LEU:HD13	1:7:A:LEU:HG	2	0.35
(1,339)	1:7:A:LEU:HD21	1:7:A:LEU:HG	2	0.35
(1,339)	1:7:A:LEU:HD22	1:7:A:LEU:HG	2	0.35
(1,339)	1:7:A:LEU:HD23	1:7:A:LEU:HG	2	0.35
(1,339)	1:7:A:LEU:HD11	1:7:A:LEU:HG	3	0.35
(1,339)	1:7:A:LEU:HD12	1:7:A:LEU:HG	3	0.35
(1,339)	1:7:A:LEU:HD13	1:7:A:LEU:HG	3	0.35
(1,339)	1:7:A:LEU:HD21	1:7:A:LEU:HG	3	0.35
(1,339)	1:7:A:LEU:HD22	1:7:A:LEU:HG	3	0.35
(1,339)	1:7:A:LEU:HD23	1:7:A:LEU:HG	3	0.35
(1,339)	1:7:A:LEU:HD11	1:7:A:LEU:HG	4	0.35
(1,339)	1:7:A:LEU:HD12	1:7:A:LEU:HG	4	0.35
(1,339)	1:7:A:LEU:HD13	1:7:A:LEU:HG	4	0.35
(1,339)	1:7:A:LEU:HD21	1:7:A:LEU:HG	4	0.35
(1,339)	1:7:A:LEU:HD22	1:7:A:LEU:HG	4	0.35
(1,339)	1:7:A:LEU:HD23	1:7:A:LEU:HG	4	0.35
(1,339)	1:7:A:LEU:HD11	1:7:A:LEU:HG	5	0.35
(1,339)	1:7:A:LEU:HD12	1:7:A:LEU:HG	5	0.35
(1,339)	1:7:A:LEU:HD13	1:7:A:LEU:HG	5	0.35
(1,339)	1:7:A:LEU:HD21	1:7:A:LEU:HG	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:7:A:LEU:HD22	1:7:A:LEU:HG	5	0.35
(1,339)	1:7:A:LEU:HD23	1:7:A:LEU:HG	5	0.35
(1,339)	1:7:A:LEU:HD11	1:7:A:LEU:HG	7	0.35
(1,339)	1:7:A:LEU:HD12	1:7:A:LEU:HG	7	0.35
(1,339)	1:7:A:LEU:HD13	1:7:A:LEU:HG	7	0.35
(1,339)	1:7:A:LEU:HD21	1:7:A:LEU:HG	7	0.35
(1,339)	1:7:A:LEU:HD22	1:7:A:LEU:HG	7	0.35
(1,339)	1:7:A:LEU:HD23	1:7:A:LEU:HG	7	0.35
(1,339)	1:7:A:LEU:HD11	1:7:A:LEU:HG	8	0.35
(1,339)	1:7:A:LEU:HD12	1:7:A:LEU:HG	8	0.35
(1,339)	1:7:A:LEU:HD13	1:7:A:LEU:HG	8	0.35
(1,339)	1:7:A:LEU:HD21	1:7:A:LEU:HG	8	0.35
(1,339)	1:7:A:LEU:HD22	1:7:A:LEU:HG	8	0.35
(1,339)	1:7:A:LEU:HD23	1:7:A:LEU:HG	8	0.35
(1,339)	1:7:A:LEU:HD11	1:7:A:LEU:HG	9	0.35
(1,339)	1:7:A:LEU:HD12	1:7:A:LEU:HG	9	0.35
(1,339)	1:7:A:LEU:HD13	1:7:A:LEU:HG	9	0.35
(1,339)	1:7:A:LEU:HD21	1:7:A:LEU:HG	9	0.35
(1,339)	1:7:A:LEU:HD22	1:7:A:LEU:HG	9	0.35
(1,339)	1:7:A:LEU:HD23	1:7:A:LEU:HG	9	0.35
(1,336)	1:7:A:LEU:HA	1:7:A:LEU:HB3	10	0.35
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	5	0.35
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	5	0.35
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	5	0.35
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	5	0.35
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	5	0.35
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	5	0.35
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	6	0.35
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	6	0.35
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	6	0.35
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	6	0.35
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	6	0.35
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	6	0.35
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	10	0.35
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	10	0.35
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	10	0.35
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	10	0.35
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	10	0.35
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	10	0.35
(1,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	7	0.35
(1,138)	1:8:A:TYR:HB2	1:9:A:ILE:H	8	0.35
(1,138)	1:8:A:TYR:HB3	1:9:A:ILE:H	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:11:A:TRP:HE1	1:19:A:SER:HG	7	0.35
(1,65)	1:18:A:SER:H	1:18:A:SER:HA	10	0.35
(1,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.35
(1,22)	1:13:A:LYS:H	1:13:A:LYS:HD2	1	0.35
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG21	1	0.35
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG22	1	0.35
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG23	1	0.35
(4,29)	1:9:A:ILE:HD11	1:10:A:GLN:H	3	0.34
(4,29)	1:9:A:ILE:HD12	1:10:A:GLN:H	3	0.34
(4,29)	1:9:A:ILE:HD13	1:10:A:GLN:H	3	0.34
(4,17)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	3	0.34
(4,17)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	4	0.34
(4,17)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	7	0.34
(4,3)	1:12:A:LEU:HD21	1:13:A:LYS:H	2	0.34
(4,3)	1:12:A:LEU:HD22	1:13:A:LYS:H	2	0.34
(4,3)	1:12:A:LEU:HD23	1:13:A:LYS:H	2	0.34
(3,351)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	2	0.34
(3,351)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	2	0.34
(3,351)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	2	0.34
(3,351)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	7	0.34
(3,351)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	7	0.34
(3,351)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	7	0.34
(3,201)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	2	0.34
(3,126)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	4	0.34
(3,100)	1:6:A:ARG:HB2	1:7:A:LEU:H	8	0.34
(3,32)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.34
(3,26)	1:10:A:GLN:H	1:10:A:GLN:HG3	9	0.34
(3,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	5	0.34
(2,383)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	2	0.34
(2,383)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	2	0.34
(2,383)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	2	0.34
(2,383)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	7	0.34
(2,383)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	7	0.34
(2,383)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	7	0.34
(2,280)	1:9:A:ILE:HD11	1:10:A:GLN:H	3	0.34
(2,280)	1:9:A:ILE:HD12	1:10:A:GLN:H	3	0.34
(2,280)	1:9:A:ILE:HD13	1:10:A:GLN:H	3	0.34
(2,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	2	0.34
(2,177)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	3	0.34
(2,177)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	4	0.34
(2,177)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	7	0.34
(2,137)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,108)	1:6:A:ARG:HB2	1:7:A:LEU:H	8	0.34
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.34
(2,30)	1:10:A:GLN:H	1:10:A:GLN:HG3	9	0.34
(2,12)	1:12:A:LEU:HD21	1:13:A:LYS:H	2	0.34
(2,12)	1:12:A:LEU:HD22	1:13:A:LYS:H	2	0.34
(2,12)	1:12:A:LEU:HD23	1:13:A:LYS:H	2	0.34
(2,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	5	0.34
(1,618)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	3	0.34
(1,541)	1:4:A:CYS:HA	1:7:A:LEU:HB2	10	0.34
(1,529)	1:11:A:TRP:HB3	1:24:A:PRO:HD2	9	0.34
(1,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	4	0.34
(1,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	4	0.34
(1,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	4	0.34
(1,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	8	0.34
(1,420)	1:18:A:SER:HA	1:18:A:SER:HB2	8	0.34
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	5	0.34
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	5	0.34
(1,384)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	5	0.34
(1,380)	1:12:A:LEU:HB3	1:12:A:LEU:HG	10	0.34
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG21	1	0.34
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG22	1	0.34
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG23	1	0.34
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG21	4	0.34
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG22	4	0.34
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG23	4	0.34
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG21	6	0.34
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG22	6	0.34
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG23	6	0.34
(1,339)	1:7:A:LEU:HD11	1:7:A:LEU:HG	6	0.34
(1,339)	1:7:A:LEU:HD12	1:7:A:LEU:HG	6	0.34
(1,339)	1:7:A:LEU:HD13	1:7:A:LEU:HG	6	0.34
(1,339)	1:7:A:LEU:HD21	1:7:A:LEU:HG	6	0.34
(1,339)	1:7:A:LEU:HD22	1:7:A:LEU:HG	6	0.34
(1,339)	1:7:A:LEU:HD23	1:7:A:LEU:HG	6	0.34
(1,336)	1:7:A:LEU:HA	1:7:A:LEU:HB3	1	0.34
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	5	0.34
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	5	0.34
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	5	0.34
(1,192)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	5	0.34
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	5	0.34
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	5	0.34
(1,192)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:23:A:PRO:HB2	1:25:A:CYS:H	4	0.34
(1,131)	1:9:A:ILE:HA	1:12:A:LEU:H	5	0.34
(1,75)	1:19:A:SER:H	1:19:A:SER:HB3	9	0.34
(1,71)	1:25:A:CYS:H	1:25:A:CYS:HB3	1	0.34
(1,65)	1:18:A:SER:H	1:18:A:SER:HA	3	0.34
(1,65)	1:18:A:SER:H	1:18:A:SER:HA	5	0.34
(1,65)	1:18:A:SER:H	1:18:A:SER:HA	9	0.34
(1,33)	1:10:A:GLN:H	1:10:A:GLN:HB2	9	0.34
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	6	0.33
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	6	0.33
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	6	0.33
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	6	0.33
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	6	0.33
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	6	0.33
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	6	0.33
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	6	0.33
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	6	0.33
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	9	0.33
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	9	0.33
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	9	0.33
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	9	0.33
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	9	0.33
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	9	0.33
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	9	0.33
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	9	0.33
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	9	0.33
(4,29)	1:9:A:ILE:HD11	1:10:A:GLN:H	1	0.33
(4,29)	1:9:A:ILE:HD12	1:10:A:GLN:H	1	0.33
(4,29)	1:9:A:ILE:HD13	1:10:A:GLN:H	1	0.33
(4,16)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	2	0.33
(4,16)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	2	0.33
(4,11)	1:12:A:LEU:H	1:13:A:LYS:HA	2	0.33
(4,3)	1:12:A:LEU:HD21	1:13:A:LYS:H	7	0.33
(4,3)	1:12:A:LEU:HD22	1:13:A:LYS:H	7	0.33
(4,3)	1:12:A:LEU:HD23	1:13:A:LYS:H	7	0.33
(3,201)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	1	0.33
(3,126)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	2	0.33
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	6	0.33
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	6	0.33
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	6	0.33
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	6	0.33
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	6	0.33
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	6	0.33
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	6	0.33
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	6	0.33
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	9	0.33
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	9	0.33
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	9	0.33
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	9	0.33
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	9	0.33
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	9	0.33
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	9	0.33
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	9	0.33
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	9	0.33
(2,280)	1:9:A:ILE:HD11	1:10:A:GLN:H	1	0.33
(2,280)	1:9:A:ILE:HD12	1:10:A:GLN:H	1	0.33
(2,280)	1:9:A:ILE:HD13	1:10:A:GLN:H	1	0.33
(2,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	1	0.33
(2,175)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	2	0.33
(2,175)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	2	0.33
(2,137)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	2	0.33
(2,132)	1:12:A:LEU:H	1:13:A:LYS:HA	2	0.33
(2,12)	1:12:A:LEU:HD21	1:13:A:LYS:H	7	0.33
(2,12)	1:12:A:LEU:HD22	1:13:A:LYS:H	7	0.33
(2,12)	1:12:A:LEU:HD23	1:13:A:LYS:H	7	0.33
(1,599)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	8	0.33
(1,599)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	8	0.33
(1,597)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	9	0.33
(1,540)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.33
(1,517)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	4	0.33
(1,503)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	2	0.33
(1,380)	1:12:A:LEU:HB3	1:12:A:LEU:HG	1	0.33
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG21	9	0.33
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG22	9	0.33
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG23	9	0.33
(1,288)	1:12:A:LEU:HA	1:16:A:GLY:H	8	0.33
(1,268)	1:8:A:TYR:H	1:24:A:PRO:HG2	5	0.33
(1,138)	1:8:A:TYR:HB2	1:9:A:ILE:H	3	0.33
(1,138)	1:8:A:TYR:HB3	1:9:A:ILE:H	3	0.33
(1,138)	1:8:A:TYR:HB2	1:9:A:ILE:H	9	0.33
(1,138)	1:8:A:TYR:HB3	1:9:A:ILE:H	9	0.33
(1,131)	1:9:A:ILE:HA	1:12:A:LEU:H	7	0.33
(1,115)	1:2:A:GLU:HB3	1:5:A:VAL:H	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:11:A:TRP:HE1	1:19:A:SER:HG	6	0.33
(1,91)	1:11:A:TRP:HE1	1:19:A:SER:HG	10	0.33
(1,65)	1:18:A:SER:H	1:18:A:SER:HA	4	0.33
(1,65)	1:18:A:SER:H	1:18:A:SER:HA	7	0.33
(1,62)	1:20:A:GLY:H	1:20:A:GLY:HA2	7	0.33
(1,33)	1:10:A:GLN:H	1:10:A:GLN:HB2	10	0.33
(1,9)	1:7:A:LEU:HD11	1:8:A:TYR:H	9	0.33
(1,9)	1:7:A:LEU:HD12	1:8:A:TYR:H	9	0.33
(1,9)	1:7:A:LEU:HD13	1:8:A:TYR:H	9	0.33
(1,9)	1:7:A:LEU:HD21	1:8:A:TYR:H	9	0.33
(1,9)	1:7:A:LEU:HD22	1:8:A:TYR:H	9	0.33
(1,9)	1:7:A:LEU:HD23	1:8:A:TYR:H	9	0.33
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	3	0.32
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	3	0.32
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	3	0.32
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	3	0.32
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	3	0.32
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	3	0.32
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	3	0.32
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	3	0.32
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	3	0.32
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	4	0.32
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	4	0.32
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	4	0.32
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	4	0.32
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	4	0.32
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	4	0.32
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	4	0.32
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	4	0.32
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	4	0.32
(4,17)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	2	0.32
(4,10)	1:10:A:GLN:HA	1:11:A:TRP:H	8	0.32
(4,10)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.32
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.32
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.32
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.32
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.32
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.32
(3,306)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.32
(3,100)	1:6:A:ARG:HB2	1:7:A:LEU:H	2	0.32
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	3	0.32
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	3	0.32
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	3	0.32
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	3	0.32
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	3	0.32
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	3	0.32
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	3	0.32
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	3	0.32
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	4	0.32
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	4	0.32
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	4	0.32
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	4	0.32
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	4	0.32
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	4	0.32
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	4	0.32
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	4	0.32
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	4	0.32
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.32
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.32
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.32
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.32
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.32
(2,337)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.32
(2,177)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	2	0.32
(2,125)	1:10:A:GLN:HA	1:11:A:TRP:H	8	0.32
(2,125)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.32
(2,108)	1:6:A:ARG:HB2	1:7:A:LEU:H	2	0.32
(1,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	5	0.32
(1,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	5	0.32
(1,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	5	0.32
(1,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	5	0.32
(1,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	5	0.32
(1,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	5	0.32
(1,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	5	0.32
(1,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	5	0.32
(1,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	5	0.32
(1,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	4	0.32
(1,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	5	0.32
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	8	0.32
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	8	0.32
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	8	0.32
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	8	0.32
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	8	0.32
(1,558)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	7	0.32
(1,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	7	0.32
(1,541)	1:4:A:CYS:HA	1:7:A:LEU:HB2	1	0.32
(1,534)	1:21:A:ARG:HB3	1:22:A:PRO:HD2	6	0.32
(1,534)	1:21:A:ARG:HB3	1:22:A:PRO:HD2	10	0.32
(1,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	2	0.32
(1,476)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	6	0.32
(1,476)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	9	0.32
(1,463)	1:21:A:ARG:HA	1:22:A:PRO:HD3	8	0.32
(1,445)	1:22:A:PRO:HA	1:22:A:PRO:HG3	3	0.32
(1,435)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	8	0.32
(1,405)	1:17:A:PRO:HA	1:17:A:PRO:HD3	1	0.32
(1,405)	1:17:A:PRO:HA	1:17:A:PRO:HD3	6	0.32
(1,390)	1:13:A:LYS:HA	1:13:A:LYS:HD2	9	0.32
(1,372)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	1	0.32
(1,372)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	2	0.32
(1,372)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	3	0.32
(1,372)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	4	0.32
(1,372)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	5	0.32
(1,372)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	6	0.32
(1,372)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	7	0.32
(1,372)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	8	0.32
(1,372)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	9	0.32
(1,372)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.32
(1,360)	1:10:A:GLN:HA	1:10:A:GLN:HG3	9	0.32
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	3	0.32
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	3	0.32
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	3	0.32
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	3	0.32
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	3	0.32
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	3	0.32
(1,328)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	2	0.32
(1,328)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.32
(1,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	6	0.32
(1,138)	1:8:A:TYR:HB2	1:9:A:ILE:H	5	0.32
(1,138)	1:8:A:TYR:HB3	1:9:A:ILE:H	5	0.32
(1,138)	1:8:A:TYR:HB2	1:9:A:ILE:H	6	0.32
(1,138)	1:8:A:TYR:HB3	1:9:A:ILE:H	6	0.32
(1,75)	1:19:A:SER:H	1:19:A:SER:HB3	3	0.32
(1,27)	1:4:A:CYS:H	1:4:A:CYS:HB3	2	0.32
(4,10)	1:10:A:GLN:HA	1:11:A:TRP:H	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,171)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	9	0.31
(3,69)	1:19:A:SER:H	1:19:A:SER:HB2	8	0.31
(3,26)	1:10:A:GLN:H	1:10:A:GLN:HG3	5	0.31
(2,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	9	0.31
(2,125)	1:10:A:GLN:HA	1:11:A:TRP:H	5	0.31
(2,76)	1:19:A:SER:H	1:19:A:SER:HB2	8	0.31
(2,30)	1:10:A:GLN:H	1:10:A:GLN:HG3	5	0.31
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	2	0.31
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	2	0.31
(1,654)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	2	0.31
(1,635)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	3	0.31
(1,635)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	3	0.31
(1,635)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	3	0.31
(1,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	10	0.31
(1,618)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	1	0.31
(1,564)	1:11:A:TRP:HA	1:14:A:ASP:HB2	7	0.31
(1,558)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	8	0.31
(1,544)	1:8:A:TYR:HA	1:24:A:PRO:HD3	2	0.31
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB2	8	0.31
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB3	8	0.31
(1,538)	1:7:A:LEU:HA	1:10:A:GLN:HB3	1	0.31
(1,531)	1:11:A:TRP:HB3	1:24:A:PRO:HG3	1	0.31
(1,528)	1:11:A:TRP:HB3	1:24:A:PRO:HD3	7	0.31
(1,503)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	4	0.31
(1,503)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	5	0.31
(1,491)	1:24:A:PRO:HA	1:24:A:PRO:HB3	4	0.31
(1,476)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	3	0.31
(1,476)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	7	0.31
(1,476)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.31
(1,463)	1:21:A:ARG:HA	1:22:A:PRO:HD3	5	0.31
(1,420)	1:18:A:SER:HA	1:18:A:SER:HB2	9	0.31
(1,380)	1:12:A:LEU:HB3	1:12:A:LEU:HG	9	0.31
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	2	0.31
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	2	0.31
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	2	0.31
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	2	0.31
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	2	0.31
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	2	0.31
(1,268)	1:8:A:TYR:H	1:24:A:PRO:HG2	6	0.31
(1,205)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	9	0.31
(1,205)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	9	0.31
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	9	0.31
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	9	0.31
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	9	0.31
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	9	0.31
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	9	0.31
(1,182)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	1	0.31
(1,182)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	1	0.31
(1,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	5	0.31
(1,145)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	7	0.31
(1,145)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	10	0.31
(1,115)	1:2:A:GLU:HB3	1:5:A:VAL:H	3	0.31
(1,102)	1:10:A:GLN:HB3	1:11:A:TRP:H	10	0.31
(1,65)	1:18:A:SER:H	1:18:A:SER:HA	2	0.31
(1,65)	1:18:A:SER:H	1:18:A:SER:HA	6	0.31
(1,62)	1:20:A:GLY:H	1:20:A:GLY:HA2	10	0.31
(1,33)	1:10:A:GLN:H	1:10:A:GLN:HB2	8	0.31
(1,27)	1:4:A:CYS:H	1:4:A:CYS:HB3	1	0.31
(4,14)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.3
(4,14)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.3
(4,14)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.3
(4,14)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.3
(4,10)	1:10:A:GLN:HA	1:11:A:TRP:H	4	0.3
(4,10)	1:10:A:GLN:HA	1:11:A:TRP:H	7	0.3
(3,612)	1:2:A:GLU:HB3	1:6:A:ARG:HA	5	0.3
(3,214)	1:15:A:GLY:HA2	1:16:A:GLY:H	5	0.3
(3,126)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	1	0.3
(3,32)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.3
(3,26)	1:10:A:GLN:H	1:10:A:GLN:HG3	7	0.3
(2,663)	1:2:A:GLU:HB3	1:6:A:ARG:HA	5	0.3
(2,239)	1:15:A:GLY:HA2	1:16:A:GLY:H	5	0.3
(2,169)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.3
(2,169)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.3
(2,169)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.3
(2,169)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.3
(2,137)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	1	0.3
(2,125)	1:10:A:GLN:HA	1:11:A:TRP:H	4	0.3
(2,125)	1:10:A:GLN:HA	1:11:A:TRP:H	7	0.3
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.3
(2,30)	1:10:A:GLN:H	1:10:A:GLN:HG3	7	0.3
(1,662)	1:6:A:ARG:HA	1:9:A:ILE:HG12	5	0.3
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG21	5	0.3
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG22	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG23	5	0.3
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	3	0.3
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	3	0.3
(1,648)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	3	0.3
(1,634)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	3	0.3
(1,634)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	3	0.3
(1,634)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	3	0.3
(1,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	7	0.3
(1,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	9	0.3
(1,569)	1:23:A:PRO:HA	1:24:A:PRO:HD3	2	0.3
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	3	0.3
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	3	0.3
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	3	0.3
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	3	0.3
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	3	0.3
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	3	0.3
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB2	1	0.3
(1,539)	1:3:A:GLU:HA	1:6:A:ARG:HB3	1	0.3
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE2	5	0.3
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE3	5	0.3
(1,503)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	1	0.3
(1,503)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	3	0.3
(1,503)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	6	0.3
(1,503)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	7	0.3
(1,491)	1:24:A:PRO:HA	1:24:A:PRO:HB3	2	0.3
(1,491)	1:24:A:PRO:HA	1:24:A:PRO:HB3	5	0.3
(1,491)	1:24:A:PRO:HA	1:24:A:PRO:HB3	6	0.3
(1,491)	1:24:A:PRO:HA	1:24:A:PRO:HB3	10	0.3
(1,476)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	1	0.3
(1,476)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	4	0.3
(1,476)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	5	0.3
(1,476)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	8	0.3
(1,463)	1:21:A:ARG:HA	1:22:A:PRO:HD3	6	0.3
(1,380)	1:12:A:LEU:HB3	1:12:A:LEU:HG	8	0.3
(1,328)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	7	0.3
(1,205)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	10	0.3
(1,205)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	10	0.3
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	10	0.3
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	10	0.3
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	10	0.3
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	10	0.3
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	10	0.3
(1,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	4	0.3
(1,138)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.3
(1,138)	1:8:A:TYR:HB3	1:9:A:ILE:H	10	0.3
(1,80)	1:5:A:VAL:HA	1:8:A:TYR:H	8	0.3
(1,64)	1:18:A:SER:H	1:18:A:SER:HB2	2	0.3
(4,28)	1:5:A:VAL:HG11	1:6:A:ARG:H	3	0.29
(4,28)	1:5:A:VAL:HG12	1:6:A:ARG:H	3	0.29
(4,28)	1:5:A:VAL:HG13	1:6:A:ARG:H	3	0.29
(4,14)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.29
(4,14)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.29
(4,14)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.29
(4,14)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.29
(4,10)	1:10:A:GLN:HA	1:11:A:TRP:H	1	0.29
(4,10)	1:10:A:GLN:HA	1:11:A:TRP:H	3	0.29
(4,10)	1:10:A:GLN:HA	1:11:A:TRP:H	6	0.29
(4,10)	1:10:A:GLN:HA	1:11:A:TRP:H	9	0.29
(3,602)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	7	0.29
(3,602)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	7	0.29
(3,602)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	7	0.29
(3,214)	1:15:A:GLY:HA2	1:16:A:GLY:H	3	0.29
(3,32)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.29
(2,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	7	0.29
(2,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	7	0.29
(2,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	7	0.29
(2,277)	1:5:A:VAL:HG11	1:6:A:ARG:H	3	0.29
(2,277)	1:5:A:VAL:HG12	1:6:A:ARG:H	3	0.29
(2,277)	1:5:A:VAL:HG13	1:6:A:ARG:H	3	0.29
(2,239)	1:15:A:GLY:HA2	1:16:A:GLY:H	3	0.29
(2,169)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.29
(2,169)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.29
(2,169)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.29
(2,169)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.29
(2,125)	1:10:A:GLN:HA	1:11:A:TRP:H	1	0.29
(2,125)	1:10:A:GLN:HA	1:11:A:TRP:H	3	0.29
(2,125)	1:10:A:GLN:HA	1:11:A:TRP:H	6	0.29
(2,125)	1:10:A:GLN:HA	1:11:A:TRP:H	9	0.29
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.29
(1,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	6	0.29
(1,619)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	8	0.29
(1,599)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	3	0.29
(1,599)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	10	0.29
(1,599)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	10	0.29
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	9	0.29
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	9	0.29
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	9	0.29
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	9	0.29
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	9	0.29
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	9	0.29
(1,558)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	4	0.29
(1,558)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	9	0.29
(1,552)	1:22:A:PRO:HA	1:23:A:PRO:HD3	6	0.29
(1,551)	1:22:A:PRO:HA	1:23:A:PRO:HD2	3	0.29
(1,529)	1:11:A:TRP:HB3	1:24:A:PRO:HD2	1	0.29
(1,529)	1:11:A:TRP:HB3	1:24:A:PRO:HD2	7	0.29
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	6	0.29
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	6	0.29
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	8	0.29
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	8	0.29
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	0.29
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	10	0.29
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE2	8	0.29
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE3	8	0.29
(1,503)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	8	0.29
(1,491)	1:24:A:PRO:HA	1:24:A:PRO:HB3	1	0.29
(1,491)	1:24:A:PRO:HA	1:24:A:PRO:HB3	3	0.29
(1,491)	1:24:A:PRO:HA	1:24:A:PRO:HB3	7	0.29
(1,491)	1:24:A:PRO:HA	1:24:A:PRO:HB3	8	0.29
(1,486)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	5	0.29
(1,400)	1:14:A:ASP:HA	1:14:A:ASP:HB2	4	0.29
(1,354)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	8	0.29
(1,354)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	8	0.29
(1,354)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	8	0.29
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	8	0.29
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	8	0.29
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	8	0.29
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	8	0.29
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	8	0.29
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	8	0.29
(1,328)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	5	0.29
(1,328)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	9	0.29
(1,303)	1:3:A:GLU:HA	1:3:A:GLU:HG2	10	0.29
(1,303)	1:3:A:GLU:HA	1:3:A:GLU:HG3	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:2:A:GLU:HA	1:2:A:GLU:HG3	4	0.29
(1,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	5	0.29
(1,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	5	0.29
(1,182)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	7	0.29
(1,182)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	7	0.29
(1,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	8	0.29
(1,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	9	0.29
(1,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	3	0.29
(1,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	6	0.29
(1,134)	1:19:A:SER:HB2	1:21:A:ARG:H	1	0.29
(1,131)	1:9:A:ILE:HA	1:12:A:LEU:H	2	0.29
(1,110)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.29
(1,105)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.29
(1,75)	1:19:A:SER:H	1:19:A:SER:HB3	10	0.29
(4,14)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.28
(4,10)	1:10:A:GLN:HA	1:11:A:TRP:H	2	0.28
(3,602)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	2	0.28
(3,602)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	2	0.28
(3,602)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	2	0.28
(3,492)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	5	0.28
(3,201)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	6	0.28
(3,189)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	9	0.28
(3,26)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.28
(2,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	2	0.28
(2,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	2	0.28
(2,653)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	2	0.28
(2,530)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	5	0.28
(2,226)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	6	0.28
(2,211)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	9	0.28
(2,169)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.28
(2,125)	1:10:A:GLN:HA	1:11:A:TRP:H	2	0.28
(2,30)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.28
(1,593)	1:2:A:GLU:HB3	1:6:A:ARG:H	2	0.28
(1,583)	1:6:A:ARG:HB3	1:7:A:LEU:H	10	0.28
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	4	0.28
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	4	0.28
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	4	0.28
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	4	0.28
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	4	0.28
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	4	0.28
(1,558)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	10	0.28
(1,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:8:A:TYR:HA	1:24:A:PRO:HD3	1	0.28
(1,544)	1:8:A:TYR:HA	1:24:A:PRO:HD3	4	0.28
(1,544)	1:8:A:TYR:HA	1:24:A:PRO:HD3	5	0.28
(1,544)	1:8:A:TYR:HA	1:24:A:PRO:HD3	6	0.28
(1,544)	1:8:A:TYR:HA	1:24:A:PRO:HD3	9	0.28
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	2	0.28
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	2	0.28
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	5	0.28
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	5	0.28
(1,503)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.28
(1,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	4	0.28
(1,486)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	1	0.28
(1,486)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	4	0.28
(1,463)	1:21:A:ARG:HA	1:22:A:PRO:HD3	4	0.28
(1,445)	1:22:A:PRO:HA	1:22:A:PRO:HG3	2	0.28
(1,425)	1:19:A:SER:HB2	1:19:A:SER:HB3	8	0.28
(1,420)	1:18:A:SER:HA	1:18:A:SER:HB2	1	0.28
(1,404)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	6	0.28
(1,404)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	8	0.28
(1,404)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	9	0.28
(1,404)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.28
(1,400)	1:14:A:ASP:HA	1:14:A:ASP:HB2	5	0.28
(1,354)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	1	0.28
(1,354)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	1	0.28
(1,354)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	1	0.28
(1,354)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	3	0.28
(1,354)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	3	0.28
(1,354)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	3	0.28
(1,354)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	4	0.28
(1,354)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	4	0.28
(1,354)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	4	0.28
(1,354)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	6	0.28
(1,354)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	6	0.28
(1,354)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	6	0.28
(1,354)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	9	0.28
(1,354)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	9	0.28
(1,354)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	9	0.28
(1,354)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	10	0.28
(1,354)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	10	0.28
(1,354)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	10	0.28
(1,352)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	3	0.28
(1,352)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	8	0.28
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	5	0.28
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	5	0.28
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	5	0.28
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	5	0.28
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	5	0.28
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	5	0.28
(1,304)	1:3:A:GLU:HA	1:3:A:GLU:HB2	9	0.28
(1,304)	1:3:A:GLU:HA	1:3:A:GLU:HB3	9	0.28
(1,205)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	7	0.28
(1,205)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	7	0.28
(1,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	6	0.28
(1,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	6	0.28
(1,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	8	0.28
(1,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	8	0.28
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	6	0.28
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	6	0.28
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	6	0.28
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	6	0.28
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	6	0.28
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	6	0.28
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	6	0.28
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	6	0.28
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	6	0.28
(1,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	6	0.28
(1,143)	1:23:A:PRO:HB2	1:25:A:CYS:H	3	0.28
(1,91)	1:11:A:TRP:HE1	1:19:A:SER:HG	3	0.28
(1,91)	1:11:A:TRP:HE1	1:19:A:SER:HG	5	0.28
(1,80)	1:5:A:VAL:HA	1:8:A:TYR:H	2	0.28
(1,75)	1:19:A:SER:H	1:19:A:SER:HB3	4	0.28
(1,75)	1:19:A:SER:H	1:19:A:SER:HB3	5	0.28
(1,75)	1:19:A:SER:H	1:19:A:SER:HB3	6	0.28
(1,62)	1:20:A:GLY:H	1:20:A:GLY:HA2	3	0.28
(1,22)	1:13:A:LYS:H	1:13:A:LYS:HD2	5	0.28
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	5	0.27
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	5	0.27
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	5	0.27
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	5	0.27
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	5	0.27
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	5	0.27
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	5	0.27
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	5	0.27
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD11	5	0.27
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD12	5	0.27
(4,39)	1:5:A:VAL:HA	1:9:A:ILE:HD13	5	0.27
(4,22)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	10	0.27
(4,14)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.27
(3,492)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	7	0.27
(3,32)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.27
(3,32)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.27
(3,26)	1:10:A:GLN:H	1:10:A:GLN:HG3	1	0.27
(3,26)	1:10:A:GLN:H	1:10:A:GLN:HG3	4	0.27
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	5	0.27
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	5	0.27
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	5	0.27
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	5	0.27
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	5	0.27
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	5	0.27
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	5	0.27
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	5	0.27
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	5	0.27
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD11	5	0.27
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD12	5	0.27
(2,557)	1:5:A:VAL:HA	1:9:A:ILE:HD13	5	0.27
(2,530)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	7	0.27
(2,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	10	0.27
(2,169)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.27
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.27
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.27
(2,30)	1:10:A:GLN:H	1:10:A:GLN:HG3	1	0.27
(2,30)	1:10:A:GLN:H	1:10:A:GLN:HG3	4	0.27
(1,599)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	1	0.27
(1,599)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	1	0.27
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	1	0.27
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	1	0.27
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	1	0.27
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	1	0.27
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	1	0.27
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	1	0.27
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	6	0.27
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	6	0.27
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	6	0.27
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	6	0.27
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	6	0.27
(1,558)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	3	0.27
(1,552)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.27
(1,550)	1:8:A:TYR:HA	1:11:A:TRP:HB3	2	0.27
(1,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	1	0.27
(1,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	10	0.27
(1,531)	1:11:A:TRP:HB3	1:24:A:PRO:HG3	8	0.27
(1,531)	1:11:A:TRP:HB3	1:24:A:PRO:HG3	9	0.27
(1,528)	1:11:A:TRP:HB3	1:24:A:PRO:HD3	1	0.27
(1,528)	1:11:A:TRP:HB3	1:24:A:PRO:HD3	10	0.27
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	1	0.27
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	1	0.27
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	3	0.27
(1,521)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	3	0.27
(1,503)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	9	0.27
(1,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	5	0.27
(1,491)	1:24:A:PRO:HA	1:24:A:PRO:HB3	9	0.27
(1,486)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	3	0.27
(1,486)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	8	0.27
(1,486)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	10	0.27
(1,469)	1:23:A:PRO:HA	1:23:A:PRO:HD3	7	0.27
(1,405)	1:17:A:PRO:HA	1:17:A:PRO:HD3	2	0.27
(1,404)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	1	0.27
(1,404)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	2	0.27
(1,404)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	3	0.27
(1,404)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	4	0.27
(1,404)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	5	0.27
(1,404)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	7	0.27
(1,400)	1:14:A:ASP:HA	1:14:A:ASP:HB2	2	0.27
(1,400)	1:14:A:ASP:HA	1:14:A:ASP:HB2	9	0.27
(1,379)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	1	0.27
(1,379)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	2	0.27
(1,379)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	3	0.27
(1,379)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	4	0.27
(1,379)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	5	0.27
(1,379)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	6	0.27
(1,379)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	7	0.27
(1,379)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	9	0.27
(1,379)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.27
(1,354)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	5	0.27
(1,354)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	5	0.27
(1,352)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	1	0.27
(1,352)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	2	0.27
(1,352)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	5	0.27
(1,352)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	6	0.27
(1,352)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	9	0.27
(1,352)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	10	0.27
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.27
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.27
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.27
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	6	0.27
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	6	0.27
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	6	0.27
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	7	0.27
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	7	0.27
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	7	0.27
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	7	0.27
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	7	0.27
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	7	0.27
(1,297)	1:2:A:GLU:HA	1:2:A:GLU:HG2	9	0.27
(1,258)	1:14:A:ASP:HB3	1:16:A:GLY:H	6	0.27
(1,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	5	0.27
(1,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	3	0.27
(1,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	3	0.27
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	3	0.27
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	3	0.27
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	3	0.27
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	3	0.27
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	3	0.27
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	3	0.27
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	3	0.27
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	3	0.27
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	3	0.27
(1,138)	1:8:A:TYR:HB2	1:9:A:ILE:H	1	0.27
(1,138)	1:8:A:TYR:HB3	1:9:A:ILE:H	1	0.27
(1,138)	1:8:A:TYR:HB2	1:9:A:ILE:H	4	0.27
(1,138)	1:8:A:TYR:HB3	1:9:A:ILE:H	4	0.27
(1,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	2	0.27
(1,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.27
(1,27)	1:4:A:CYS:H	1:4:A:CYS:HB3	10	0.27
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	8	0.26
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	8	0.26
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	8	0.26
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	8	0.26
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	8	0.26
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	8	0.26
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	8	0.26
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	8	0.26
(4,4)	1:9:A:ILE:HG21	1:10:A:GLN:H	4	0.26
(4,4)	1:9:A:ILE:HG22	1:10:A:GLN:H	4	0.26
(4,4)	1:9:A:ILE:HG23	1:10:A:GLN:H	4	0.26
(3,542)	1:6:A:ARG:HB3	1:7:A:LEU:H	7	0.26
(3,492)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	4	0.26
(3,492)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	6	0.26
(3,492)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	8	0.26
(3,492)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	10	0.26
(3,214)	1:15:A:GLY:HA2	1:16:A:GLY:H	1	0.26
(3,198)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	1	0.26
(3,198)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	1	0.26
(3,195)	1:8:A:TYR:HE1	1:12:A:LEU:HG	1	0.26
(3,195)	1:8:A:TYR:HE2	1:12:A:LEU:HG	1	0.26
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG2	6	0.26
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	8	0.26
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	8	0.26
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	8	0.26
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	8	0.26
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	8	0.26
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	8	0.26
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	8	0.26
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	8	0.26
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	8	0.26
(2,583)	1:6:A:ARG:HB3	1:7:A:LEU:H	7	0.26
(2,530)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	4	0.26
(2,530)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	6	0.26
(2,530)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	8	0.26
(2,530)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	10	0.26
(2,239)	1:15:A:GLY:HA2	1:16:A:GLY:H	1	0.26
(2,223)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	1	0.26
(2,223)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	1	0.26
(2,219)	1:8:A:TYR:HE1	1:12:A:LEU:HG	1	0.26
(2,219)	1:8:A:TYR:HE2	1:12:A:LEU:HG	1	0.26
(2,18)	1:6:A:ARG:H	1:6:A:ARG:HG2	6	0.26
(2,15)	1:9:A:ILE:HG21	1:10:A:GLN:H	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:9:A:ILE:HG22	1:10:A:GLN:H	4	0.26
(2,15)	1:9:A:ILE:HG23	1:10:A:GLN:H	4	0.26
(1,635)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	6	0.26
(1,635)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	6	0.26
(1,635)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	6	0.26
(1,602)	1:8:A:TYR:HD1	1:25:A:CYS:HB2	2	0.26
(1,602)	1:8:A:TYR:HD2	1:25:A:CYS:HB2	2	0.26
(1,599)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	7	0.26
(1,599)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	7	0.26
(1,583)	1:6:A:ARG:HB3	1:7:A:LEU:H	3	0.26
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.26
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.26
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.26
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	10	0.26
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	10	0.26
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	10	0.26
(1,551)	1:22:A:PRO:HA	1:23:A:PRO:HD2	7	0.26
(1,547)	1:14:A:ASP:HB2	1:19:A:SER:HB3	6	0.26
(1,544)	1:8:A:TYR:HA	1:24:A:PRO:HD3	3	0.26
(1,529)	1:11:A:TRP:HB3	1:24:A:PRO:HD2	4	0.26
(1,529)	1:11:A:TRP:HB3	1:24:A:PRO:HD2	5	0.26
(1,528)	1:11:A:TRP:HB3	1:24:A:PRO:HD3	3	0.26
(1,528)	1:11:A:TRP:HB3	1:24:A:PRO:HD3	8	0.26
(1,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	1	0.26
(1,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	6	0.26
(1,486)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	6	0.26
(1,486)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	7	0.26
(1,486)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	9	0.26
(1,463)	1:21:A:ARG:HA	1:22:A:PRO:HD3	10	0.26
(1,425)	1:19:A:SER:HB2	1:19:A:SER:HB3	1	0.26
(1,425)	1:19:A:SER:HB2	1:19:A:SER:HB3	2	0.26
(1,425)	1:19:A:SER:HB2	1:19:A:SER:HB3	4	0.26
(1,425)	1:19:A:SER:HB2	1:19:A:SER:HB3	5	0.26
(1,425)	1:19:A:SER:HB2	1:19:A:SER:HB3	9	0.26
(1,379)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	8	0.26
(1,354)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	7	0.26
(1,354)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	7	0.26
(1,354)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	7	0.26
(1,352)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	7	0.26
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG21	5	0.26
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG22	5	0.26
(1,348)	1:9:A:ILE:HA	1:9:A:ILE:HG23	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	4	0.26
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	4	0.26
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	4	0.26
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	4	0.26
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	4	0.26
(1,338)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	4	0.26
(1,333)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	3	0.26
(1,328)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	4	0.26
(1,300)	1:2:A:GLU:HB3	1:2:A:GLU:HG2	4	0.26
(1,258)	1:14:A:ASP:HB3	1:16:A:GLY:H	7	0.26
(1,258)	1:14:A:ASP:HB3	1:16:A:GLY:H	10	0.26
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	8	0.26
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	8	0.26
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	8	0.26
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	8	0.26
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	8	0.26
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	8	0.26
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	1	0.26
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	1	0.26
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	1	0.26
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	10	0.26
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	10	0.26
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	10	0.26
(1,188)	1:11:A:TRP:HE3	1:16:A:GLY:HA3	2	0.26
(1,91)	1:11:A:TRP:HE1	1:19:A:SER:HG	9	0.26
(1,62)	1:20:A:GLY:H	1:20:A:GLY:HA2	9	0.26
(1,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.26
(1,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	8	0.26
(1,27)	1:4:A:CYS:H	1:4:A:CYS:HB3	4	0.26
(4,28)	1:5:A:VAL:HG11	1:6:A:ARG:H	1	0.25
(4,28)	1:5:A:VAL:HG12	1:6:A:ARG:H	1	0.25
(4,28)	1:5:A:VAL:HG13	1:6:A:ARG:H	1	0.25
(4,4)	1:9:A:ILE:HG21	1:10:A:GLN:H	10	0.25
(4,4)	1:9:A:ILE:HG22	1:10:A:GLN:H	10	0.25
(4,4)	1:9:A:ILE:HG23	1:10:A:GLN:H	10	0.25
(3,492)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	9	0.25
(3,431)	1:23:A:PRO:HA	1:23:A:PRO:HG2	2	0.25
(3,361)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	1	0.25
(3,231)	1:10:A:GLN:HG2	1:11:A:TRP:H	4	0.25
(2,530)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	9	0.25
(2,465)	1:23:A:PRO:HA	1:23:A:PRO:HG2	2	0.25
(2,394)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,277)	1:5:A:VAL:HG11	1:6:A:ARG:H	1	0.25
(2,277)	1:5:A:VAL:HG12	1:6:A:ARG:H	1	0.25
(2,277)	1:5:A:VAL:HG13	1:6:A:ARG:H	1	0.25
(2,256)	1:10:A:GLN:HG2	1:11:A:TRP:H	4	0.25
(2,15)	1:9:A:ILE:HG21	1:10:A:GLN:H	10	0.25
(2,15)	1:9:A:ILE:HG22	1:10:A:GLN:H	10	0.25
(2,15)	1:9:A:ILE:HG23	1:10:A:GLN:H	10	0.25
(1,552)	1:22:A:PRO:HA	1:23:A:PRO:HD3	5	0.25
(1,544)	1:8:A:TYR:HA	1:24:A:PRO:HD3	10	0.25
(1,529)	1:11:A:TRP:HB3	1:24:A:PRO:HD2	3	0.25
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE2	3	0.25
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE3	3	0.25
(1,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	3	0.25
(1,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	7	0.25
(1,469)	1:23:A:PRO:HA	1:23:A:PRO:HD3	3	0.25
(1,463)	1:21:A:ARG:HA	1:22:A:PRO:HD3	9	0.25
(1,425)	1:19:A:SER:HB2	1:19:A:SER:HB3	3	0.25
(1,425)	1:19:A:SER:HB2	1:19:A:SER:HB3	6	0.25
(1,425)	1:19:A:SER:HB2	1:19:A:SER:HB3	7	0.25
(1,425)	1:19:A:SER:HB2	1:19:A:SER:HB3	10	0.25
(1,420)	1:18:A:SER:HA	1:18:A:SER:HB2	2	0.25
(1,407)	1:17:A:PRO:HA	1:17:A:PRO:HB3	2	0.25
(1,400)	1:14:A:ASP:HA	1:14:A:ASP:HB2	1	0.25
(1,400)	1:14:A:ASP:HA	1:14:A:ASP:HB2	3	0.25
(1,360)	1:10:A:GLN:HA	1:10:A:GLN:HG3	8	0.25
(1,354)	1:9:A:ILE:HD11	1:9:A:ILE:HG12	2	0.25
(1,354)	1:9:A:ILE:HD12	1:9:A:ILE:HG12	2	0.25
(1,354)	1:9:A:ILE:HD13	1:9:A:ILE:HG12	2	0.25
(1,333)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	4	0.25
(1,333)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	6	0.25
(1,333)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	9	0.25
(1,328)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	6	0.25
(1,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	1	0.25
(1,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	5	0.25
(1,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.25
(1,110)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.25
(1,105)	1:7:A:LEU:H	1:7:A:LEU:HG	1	0.25
(1,91)	1:11:A:TRP:HE1	1:19:A:SER:HG	2	0.25
(1,87)	1:19:A:SER:H	1:19:A:SER:HG	2	0.25
(1,81)	1:4:A:CYS:HA	1:7:A:LEU:H	9	0.25
(1,80)	1:5:A:VAL:HA	1:8:A:TYR:H	4	0.25
(1,72)	1:25:A:CYS:H	1:25:A:CYS:HB2	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:20:A:GLY:H	1:20:A:GLY:HA2	5	0.25
(1,62)	1:20:A:GLY:H	1:20:A:GLY:HA2	6	0.25
(1,41)	1:14:A:ASP:H	1:14:A:ASP:HB2	8	0.25
(1,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	0.25
(1,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	6	0.25
(1,27)	1:4:A:CYS:H	1:4:A:CYS:HB3	8	0.25
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG21	5	0.25
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG22	5	0.25
(1,8)	1:5:A:VAL:H	1:5:A:VAL:HG23	5	0.25
(4,27)	1:12:A:LEU:H	1:12:A:LEU:HB3	7	0.24
(4,4)	1:9:A:ILE:HG21	1:10:A:GLN:H	6	0.24
(4,4)	1:9:A:ILE:HG22	1:10:A:GLN:H	6	0.24
(4,4)	1:9:A:ILE:HG23	1:10:A:GLN:H	6	0.24
(4,4)	1:9:A:ILE:HG21	1:10:A:GLN:H	9	0.24
(4,4)	1:9:A:ILE:HG22	1:10:A:GLN:H	9	0.24
(4,4)	1:9:A:ILE:HG23	1:10:A:GLN:H	9	0.24
(3,600)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	2	0.24
(3,600)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	2	0.24
(3,600)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	2	0.24
(3,600)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	7	0.24
(3,600)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	7	0.24
(3,600)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	7	0.24
(3,299)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	7	0.24
(3,214)	1:15:A:GLY:HA2	1:16:A:GLY:H	2	0.24
(3,214)	1:15:A:GLY:HA2	1:16:A:GLY:H	9	0.24
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	4	0.24
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	4	0.24
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	4	0.24
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	4	0.24
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	4	0.24
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	4	0.24
(3,27)	1:10:A:GLN:H	1:10:A:GLN:HB3	2	0.24
(3,26)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.24
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	2	0.24
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	2	0.24
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	2	0.24
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	7	0.24
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	7	0.24
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	7	0.24
(2,330)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	7	0.24
(2,273)	1:12:A:LEU:H	1:12:A:LEU:HB3	7	0.24
(2,239)	1:15:A:GLY:HA2	1:16:A:GLY:H	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,239)	1:15:A:GLY:HA2	1:16:A:GLY:H	9	0.24
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	4	0.24
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	4	0.24
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	4	0.24
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	4	0.24
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	4	0.24
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	4	0.24
(2,32)	1:10:A:GLN:H	1:10:A:GLN:HB3	2	0.24
(2,30)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.24
(2,15)	1:9:A:ILE:HG21	1:10:A:GLN:H	6	0.24
(2,15)	1:9:A:ILE:HG22	1:10:A:GLN:H	6	0.24
(2,15)	1:9:A:ILE:HG23	1:10:A:GLN:H	6	0.24
(2,15)	1:9:A:ILE:HG21	1:10:A:GLN:H	9	0.24
(2,15)	1:9:A:ILE:HG22	1:10:A:GLN:H	9	0.24
(2,15)	1:9:A:ILE:HG23	1:10:A:GLN:H	9	0.24
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	9	0.24
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	9	0.24
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	9	0.24
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	9	0.24
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	9	0.24
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	9	0.24
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	9	0.24
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	9	0.24
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	9	0.24
(1,592)	1:2:A:GLU:HB2	1:6:A:ARG:H	2	0.24
(1,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	1	0.24
(1,552)	1:22:A:PRO:HA	1:23:A:PRO:HD3	9	0.24
(1,551)	1:22:A:PRO:HA	1:23:A:PRO:HD2	10	0.24
(1,544)	1:8:A:TYR:HA	1:24:A:PRO:HD3	7	0.24
(1,544)	1:8:A:TYR:HA	1:24:A:PRO:HD3	8	0.24
(1,540)	1:7:A:LEU:HA	1:10:A:GLN:HB2	9	0.24
(1,528)	1:11:A:TRP:HB3	1:24:A:PRO:HD3	6	0.24
(1,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	8	0.24
(1,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	10	0.24
(1,471)	1:11:A:TRP:HH2	1:23:A:PRO:HD3	9	0.24
(1,459)	1:22:A:PRO:HB3	1:22:A:PRO:HG3	1	0.24
(1,459)	1:22:A:PRO:HB3	1:22:A:PRO:HG3	2	0.24
(1,407)	1:17:A:PRO:HA	1:17:A:PRO:HB3	1	0.24
(1,407)	1:17:A:PRO:HA	1:17:A:PRO:HB3	6	0.24
(1,400)	1:14:A:ASP:HA	1:14:A:ASP:HB2	10	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	2	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	2	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	2	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	2	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	2	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	3	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	3	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	3	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	7	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	7	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	7	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	7	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	7	0.24
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	7	0.24
(1,333)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	1	0.24
(1,333)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	2	0.24
(1,333)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	5	0.24
(1,333)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	7	0.24
(1,333)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	8	0.24
(1,333)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.24
(1,328)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	1	0.24
(1,328)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	8	0.24
(1,323)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	3	0.24
(1,317)	1:6:A:ARG:HA	1:6:A:ARG:HB3	7	0.24
(1,303)	1:3:A:GLU:HA	1:3:A:GLU:HG2	7	0.24
(1,303)	1:3:A:GLU:HA	1:3:A:GLU:HG3	7	0.24
(1,297)	1:2:A:GLU:HA	1:2:A:GLU:HG2	6	0.24
(1,297)	1:2:A:GLU:HA	1:2:A:GLU:HG2	7	0.24
(1,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	1	0.24
(1,205)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	3	0.24
(1,205)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	3	0.24
(1,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.24
(1,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	8	0.24
(1,145)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	9	0.24
(1,105)	1:7:A:LEU:H	1:7:A:LEU:HG	6	0.24
(1,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.24
(1,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	9	0.24
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	8	0.23
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	8	0.23
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	8	0.23
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	8	0.23
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	8	0.23
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	8	0.23
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	8	0.23
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	8	0.23
(4,28)	1:5:A:VAL:HG11	1:6:A:ARG:H	4	0.23
(4,28)	1:5:A:VAL:HG12	1:6:A:ARG:H	4	0.23
(4,28)	1:5:A:VAL:HG13	1:6:A:ARG:H	4	0.23
(4,28)	1:5:A:VAL:HG11	1:6:A:ARG:H	6	0.23
(4,28)	1:5:A:VAL:HG12	1:6:A:ARG:H	6	0.23
(4,28)	1:5:A:VAL:HG13	1:6:A:ARG:H	6	0.23
(4,28)	1:5:A:VAL:HG11	1:6:A:ARG:H	10	0.23
(4,28)	1:5:A:VAL:HG12	1:6:A:ARG:H	10	0.23
(4,28)	1:5:A:VAL:HG13	1:6:A:ARG:H	10	0.23
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.23
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.23
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.23
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.23
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.23
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.23
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.23
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.23
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.23
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.23
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.23
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.23
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.23
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.23
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.23
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.23
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.23
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.23
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.23
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.23
(4,4)	1:9:A:ILE:HG21	1:10:A:GLN:H	8	0.23
(4,4)	1:9:A:ILE:HG22	1:10:A:GLN:H	8	0.23
(4,4)	1:9:A:ILE:HG23	1:10:A:GLN:H	8	0.23
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG11	1	0.23
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG12	1	0.23
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG13	1	0.23
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG11	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG12	10	0.23
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG13	10	0.23
(3,600)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	5	0.23
(3,600)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	5	0.23
(3,600)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	5	0.23
(3,299)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	3	0.23
(3,299)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	6	0.23
(3,231)	1:10:A:GLN:HG2	1:11:A:TRP:H	7	0.23
(3,214)	1:15:A:GLY:HA2	1:16:A:GLY:H	7	0.23
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	8	0.23
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	8	0.23
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	8	0.23
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	8	0.23
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	8	0.23
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	8	0.23
(3,26)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.23
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.23
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	5	0.23
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	5	0.23
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	5	0.23
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	8	0.23
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	8	0.23
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	8	0.23
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	8	0.23
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	8	0.23
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	8	0.23
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	8	0.23
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	8	0.23
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	8	0.23
(2,330)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	3	0.23
(2,330)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	6	0.23
(2,277)	1:5:A:VAL:HG11	1:6:A:ARG:H	4	0.23
(2,277)	1:5:A:VAL:HG12	1:6:A:ARG:H	4	0.23
(2,277)	1:5:A:VAL:HG13	1:6:A:ARG:H	4	0.23
(2,277)	1:5:A:VAL:HG11	1:6:A:ARG:H	6	0.23
(2,277)	1:5:A:VAL:HG12	1:6:A:ARG:H	6	0.23
(2,277)	1:5:A:VAL:HG13	1:6:A:ARG:H	6	0.23
(2,277)	1:5:A:VAL:HG11	1:6:A:ARG:H	10	0.23
(2,277)	1:5:A:VAL:HG12	1:6:A:ARG:H	10	0.23
(2,277)	1:5:A:VAL:HG13	1:6:A:ARG:H	10	0.23
(2,256)	1:10:A:GLN:HG2	1:11:A:TRP:H	7	0.23
(2,239)	1:15:A:GLY:HA2	1:16:A:GLY:H	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	8	0.23
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	8	0.23
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	8	0.23
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	8	0.23
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	8	0.23
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	8	0.23
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.23
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.23
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.23
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.23
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.23
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.23
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.23
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.23
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.23
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.23
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.23
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.23
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.23
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.23
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.23
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.23
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.23
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.23
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.23
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.23
(2,30)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.23
(2,18)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.23
(2,15)	1:9:A:ILE:HG21	1:10:A:GLN:H	8	0.23
(2,15)	1:9:A:ILE:HG22	1:10:A:GLN:H	8	0.23
(2,15)	1:9:A:ILE:HG23	1:10:A:GLN:H	8	0.23
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG11	1	0.23
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG12	1	0.23
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG13	1	0.23
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG11	10	0.23
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG12	10	0.23
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG13	10	0.23
(1,552)	1:22:A:PRO:HA	1:23:A:PRO:HD3	3	0.23
(1,552)	1:22:A:PRO:HA	1:23:A:PRO:HD3	4	0.23
(1,551)	1:22:A:PRO:HA	1:23:A:PRO:HD2	4	0.23
(1,551)	1:22:A:PRO:HA	1:23:A:PRO:HD2	6	0.23
(1,551)	1:22:A:PRO:HA	1:23:A:PRO:HD2	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE2	4	0.23
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE3	4	0.23
(1,497)	1:24:A:PRO:HB2	1:24:A:PRO:HD3	9	0.23
(1,471)	1:11:A:TRP:HH2	1:23:A:PRO:HD3	3	0.23
(1,471)	1:11:A:TRP:HH2	1:23:A:PRO:HD3	7	0.23
(1,469)	1:23:A:PRO:HA	1:23:A:PRO:HD3	1	0.23
(1,469)	1:23:A:PRO:HA	1:23:A:PRO:HD3	8	0.23
(1,459)	1:22:A:PRO:HB3	1:22:A:PRO:HG3	3	0.23
(1,459)	1:22:A:PRO:HB3	1:22:A:PRO:HG3	8	0.23
(1,445)	1:22:A:PRO:HA	1:22:A:PRO:HG3	1	0.23
(1,407)	1:17:A:PRO:HA	1:17:A:PRO:HB3	3	0.23
(1,407)	1:17:A:PRO:HA	1:17:A:PRO:HB3	4	0.23
(1,407)	1:17:A:PRO:HA	1:17:A:PRO:HB3	7	0.23
(1,407)	1:17:A:PRO:HA	1:17:A:PRO:HB3	8	0.23
(1,407)	1:17:A:PRO:HA	1:17:A:PRO:HB3	9	0.23
(1,407)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.23
(1,362)	1:10:A:GLN:HA	1:10:A:GLN:HB2	6	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	4	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	4	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	4	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	8	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	8	0.23
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	8	0.23
(1,255)	1:2:A:GLU:HA	1:3:A:GLU:H	10	0.23
(1,222)	1:8:A:TYR:HE1	1:9:A:ILE:HG12	10	0.23
(1,222)	1:8:A:TYR:HE2	1:9:A:ILE:HG12	10	0.23
(1,205)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	4	0.23
(1,205)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	4	0.23
(1,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	10	0.23
(1,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	10	0.23
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	8	0.23
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	8	0.23
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	8	0.23
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	9	0.23
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	9	0.23
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	10	0.23
(1,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	5	0.23
(1,145)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	8	0.23
(1,91)	1:11:A:TRP:HE1	1:19:A:SER:HG	4	0.23
(1,80)	1:5:A:VAL:HA	1:8:A:TYR:H	9	0.23
(1,62)	1:20:A:GLY:H	1:20:A:GLY:HA2	4	0.23
(1,43)	1:4:A:CYS:HB3	1:5:A:VAL:H	3	0.23
(1,41)	1:14:A:ASP:H	1:14:A:ASP:HB2	6	0.23
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	5	0.22
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	5	0.22
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	5	0.22
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	5	0.22
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	5	0.22
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	5	0.22
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	5	0.22
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	5	0.22
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	5	0.22
(4,27)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.22
(4,13)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.22
(4,13)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.22
(4,4)	1:9:A:ILE:HG21	1:10:A:GLN:H	1	0.22
(4,4)	1:9:A:ILE:HG22	1:10:A:GLN:H	1	0.22
(4,4)	1:9:A:ILE:HG23	1:10:A:GLN:H	1	0.22
(4,4)	1:9:A:ILE:HG21	1:10:A:GLN:H	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,4)	1:9:A:ILE:HG22	1:10:A:GLN:H	3	0.22
(4,4)	1:9:A:ILE:HG23	1:10:A:GLN:H	3	0.22
(4,4)	1:9:A:ILE:HG21	1:10:A:GLN:H	5	0.22
(4,4)	1:9:A:ILE:HG22	1:10:A:GLN:H	5	0.22
(4,4)	1:9:A:ILE:HG23	1:10:A:GLN:H	5	0.22
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG11	6	0.22
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG12	6	0.22
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG13	6	0.22
(3,600)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	3	0.22
(3,600)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	3	0.22
(3,600)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	3	0.22
(3,600)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	9	0.22
(3,600)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	9	0.22
(3,600)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	9	0.22
(3,299)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	9	0.22
(3,250)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.22
(3,250)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.22
(3,250)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.22
(3,231)	1:10:A:GLN:HG2	1:11:A:TRP:H	5	0.22
(3,214)	1:15:A:GLY:HA2	1:16:A:GLY:H	4	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	1	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	1	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	1	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	1	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	1	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	1	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	2	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	2	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	2	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	2	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	2	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	2	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	5	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	5	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	5	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	5	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	5	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	5	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	7	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	7	0.22
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	7	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	7	0.22
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	7	0.22
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	3	0.22
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	3	0.22
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	3	0.22
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	9	0.22
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	9	0.22
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	9	0.22
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	5	0.22
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	5	0.22
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	5	0.22
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	5	0.22
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	5	0.22
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	5	0.22
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	5	0.22
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	5	0.22
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	5	0.22
(2,330)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	9	0.22
(2,278)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.22
(2,278)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.22
(2,278)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.22
(2,273)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.22
(2,256)	1:10:A:GLN:HG2	1:11:A:TRP:H	5	0.22
(2,239)	1:15:A:GLY:HA2	1:16:A:GLY:H	4	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	1	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	1	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	1	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	1	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	1	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	1	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	2	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	2	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	2	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	2	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	2	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	2	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	5	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	5	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	5	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	5	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	5	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	7	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	7	0.22
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	7	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	7	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	7	0.22
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	7	0.22
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.22
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.22
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.22
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.22
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.22
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.22
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.22
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.22
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.22
(2,165)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.22
(2,165)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.22
(2,15)	1:9:A:ILE:HG21	1:10:A:GLN:H	1	0.22
(2,15)	1:9:A:ILE:HG22	1:10:A:GLN:H	1	0.22
(2,15)	1:9:A:ILE:HG23	1:10:A:GLN:H	1	0.22
(2,15)	1:9:A:ILE:HG21	1:10:A:GLN:H	3	0.22
(2,15)	1:9:A:ILE:HG22	1:10:A:GLN:H	3	0.22
(2,15)	1:9:A:ILE:HG23	1:10:A:GLN:H	3	0.22
(2,15)	1:9:A:ILE:HG21	1:10:A:GLN:H	5	0.22
(2,15)	1:9:A:ILE:HG22	1:10:A:GLN:H	5	0.22
(2,15)	1:9:A:ILE:HG23	1:10:A:GLN:H	5	0.22
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG11	6	0.22
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG12	6	0.22
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG13	6	0.22
(1,662)	1:6:A:ARG:HA	1:9:A:ILE:HG12	7	0.22
(1,592)	1:2:A:GLU:HB2	1:6:A:ARG:H	5	0.22
(1,592)	1:2:A:GLU:HB2	1:6:A:ARG:H	7	0.22
(1,558)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:22:A:PRO:HA	1:23:A:PRO:HD3	8	0.22
(1,551)	1:22:A:PRO:HA	1:23:A:PRO:HD2	5	0.22
(1,540)	1:7:A:LEU:HA	1:10:A:GLN:HB2	7	0.22
(1,471)	1:11:A:TRP:HH2	1:23:A:PRO:HD3	1	0.22
(1,469)	1:23:A:PRO:HA	1:23:A:PRO:HD3	9	0.22
(1,459)	1:22:A:PRO:HB3	1:22:A:PRO:HG3	5	0.22
(1,459)	1:22:A:PRO:HB3	1:22:A:PRO:HG3	7	0.22
(1,407)	1:17:A:PRO:HA	1:17:A:PRO:HB3	5	0.22
(1,400)	1:14:A:ASP:HA	1:14:A:ASP:HB2	7	0.22
(1,390)	1:13:A:LYS:HA	1:13:A:LYS:HD2	3	0.22
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	1	0.22
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	1	0.22
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	1	0.22
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	1	0.22
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	1	0.22
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	1	0.22
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	1	0.22
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	1	0.22
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	1	0.22
(1,382)	1:12:A:LEU:HD11	1:12:A:LEU:HG	8	0.22
(1,382)	1:12:A:LEU:HD12	1:12:A:LEU:HG	8	0.22
(1,382)	1:12:A:LEU:HD13	1:12:A:LEU:HG	8	0.22
(1,382)	1:12:A:LEU:HD11	1:12:A:LEU:HG	9	0.22
(1,382)	1:12:A:LEU:HD12	1:12:A:LEU:HG	9	0.22
(1,382)	1:12:A:LEU:HD13	1:12:A:LEU:HG	9	0.22
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.22
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.22
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.22
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	5	0.22
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	5	0.22
(1,343)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	5	0.22
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG11	3	0.22
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG12	3	0.22
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG13	3	0.22
(1,268)	1:8:A:TYR:H	1:24:A:PRO:HG2	7	0.22
(1,258)	1:14:A:ASP:HB3	1:16:A:GLY:H	8	0.22
(1,255)	1:2:A:GLU:HA	1:3:A:GLU:H	4	0.22
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	7	0.22
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	7	0.22
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	7	0.22
(1,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	4	0.22
(1,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	7	0.22
(1,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	2	0.22
(1,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	4	0.22
(1,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	7	0.22
(1,145)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	3	0.22
(1,131)	1:9:A:ILE:HA	1:12:A:LEU:H	4	0.22
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	3	0.22
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	8	0.22
(1,80)	1:5:A:VAL:HA	1:8:A:TYR:H	1	0.22
(1,71)	1:25:A:CYS:H	1:25:A:CYS:HB3	7	0.22
(1,62)	1:20:A:GLY:H	1:20:A:GLY:HA2	2	0.22
(1,38)	1:6:A:ARG:H	1:6:A:ARG:HB2	4	0.22
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	6	0.21
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	6	0.21
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	6	0.21
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	6	0.21
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	6	0.21
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	6	0.21
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	6	0.21
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	6	0.21
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	6	0.21
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	9	0.21
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	9	0.21
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	9	0.21
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	9	0.21
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	9	0.21
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	9	0.21
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	9	0.21
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	9	0.21
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	9	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG11	4	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG12	4	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG13	4	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG11	8	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG12	8	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG13	8	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG11	9	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG12	9	0.21
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG13	9	0.21
(3,600)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	0.21
(3,600)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	0.21
(3,600)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,567)	1:15:A:GLY:HA3	1:18:A:SER:HB3	4	0.21
(3,299)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	4	0.21
(3,250)	1:5:A:VAL:HG21	1:6:A:ARG:H	1	0.21
(3,250)	1:5:A:VAL:HG22	1:6:A:ARG:H	1	0.21
(3,250)	1:5:A:VAL:HG23	1:6:A:ARG:H	1	0.21
(3,198)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	4	0.21
(3,198)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	4	0.21
(3,189)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.21
(3,108)	1:24:A:PRO:HG3	1:25:A:CYS:H	5	0.21
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.21
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG2	9	0.21
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	0.21
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	0.21
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	0.21
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	6	0.21
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	6	0.21
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	6	0.21
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	6	0.21
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	6	0.21
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	6	0.21
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	6	0.21
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	6	0.21
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	6	0.21
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	9	0.21
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	9	0.21
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	9	0.21
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	9	0.21
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	9	0.21
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	9	0.21
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	9	0.21
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	9	0.21
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	9	0.21
(2,611)	1:15:A:GLY:HA3	1:18:A:SER:HB3	4	0.21
(2,330)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	4	0.21
(2,278)	1:5:A:VAL:HG21	1:6:A:ARG:H	1	0.21
(2,278)	1:5:A:VAL:HG22	1:6:A:ARG:H	1	0.21
(2,278)	1:5:A:VAL:HG23	1:6:A:ARG:H	1	0.21
(2,223)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	4	0.21
(2,223)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	4	0.21
(2,211)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.21
(2,117)	1:24:A:PRO:HG3	1:25:A:CYS:H	5	0.21
(2,18)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,18)	1:6:A:ARG:H	1:6:A:ARG:HG2	9	0.21
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG11	4	0.21
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG12	4	0.21
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG13	4	0.21
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG11	8	0.21
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG12	8	0.21
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG13	8	0.21
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG11	9	0.21
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG12	9	0.21
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG13	9	0.21
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	1	0.21
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	1	0.21
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	1	0.21
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	1	0.21
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	1	0.21
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	1	0.21
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	1	0.21
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	1	0.21
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	1	0.21
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	8	0.21
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	8	0.21
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	8	0.21
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	8	0.21
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	8	0.21
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	8	0.21
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	8	0.21
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	8	0.21
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	8	0.21
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB2	5	0.21
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB3	5	0.21
(1,558)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	6	0.21
(1,552)	1:22:A:PRO:HA	1:23:A:PRO:HD3	7	0.21
(1,551)	1:22:A:PRO:HA	1:23:A:PRO:HD2	1	0.21
(1,551)	1:22:A:PRO:HA	1:23:A:PRO:HD2	8	0.21
(1,531)	1:11:A:TRP:HB3	1:24:A:PRO:HG3	6	0.21
(1,471)	1:11:A:TRP:HH2	1:23:A:PRO:HD3	4	0.21
(1,471)	1:11:A:TRP:HH2	1:23:A:PRO:HD3	6	0.21
(1,471)	1:11:A:TRP:HH2	1:23:A:PRO:HD3	8	0.21
(1,471)	1:11:A:TRP:HH2	1:23:A:PRO:HD3	10	0.21
(1,469)	1:23:A:PRO:HA	1:23:A:PRO:HD3	4	0.21
(1,459)	1:22:A:PRO:HB3	1:22:A:PRO:HG3	4	0.21
(1,459)	1:22:A:PRO:HB3	1:22:A:PRO:HG3	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:22:A:PRO:HB3	1:22:A:PRO:HG3	9	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	1	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	1	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	4	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	4	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	5	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	5	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	6	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	6	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	7	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	7	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	8	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	8	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	9	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	9	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.21
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	10	0.21
(1,400)	1:14:A:ASP:HA	1:14:A:ASP:HB2	6	0.21
(1,382)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.21
(1,382)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.21
(1,382)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.21
(1,381)	1:12:A:LEU:HD21	1:12:A:LEU:HG	8	0.21
(1,381)	1:12:A:LEU:HD22	1:12:A:LEU:HG	8	0.21
(1,381)	1:12:A:LEU:HD23	1:12:A:LEU:HG	8	0.21
(1,362)	1:10:A:GLN:HA	1:10:A:GLN:HB2	1	0.21
(1,306)	1:4:A:CYS:HA	1:4:A:CYS:HB2	2	0.21
(1,306)	1:4:A:CYS:HA	1:4:A:CYS:HB2	4	0.21
(1,304)	1:3:A:GLU:HA	1:3:A:GLU:HB2	4	0.21
(1,304)	1:3:A:GLU:HA	1:3:A:GLU:HB3	4	0.21
(1,303)	1:3:A:GLU:HA	1:3:A:GLU:HG2	8	0.21
(1,303)	1:3:A:GLU:HA	1:3:A:GLU:HG3	8	0.21
(1,297)	1:2:A:GLU:HA	1:2:A:GLU:HG2	1	0.21
(1,268)	1:8:A:TYR:H	1:24:A:PRO:HG2	9	0.21
(1,255)	1:2:A:GLU:HA	1:3:A:GLU:H	8	0.21
(1,205)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	5	0.21
(1,205)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	5	0.21
(1,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	7	0.21
(1,164)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	2	0.21
(1,131)	1:9:A:ILE:HA	1:12:A:LEU:H	9	0.21
(1,80)	1:5:A:VAL:HA	1:8:A:TYR:H	3	0.21
(1,75)	1:19:A:SER:H	1:19:A:SER:HB3	7	0.21
(1,41)	1:14:A:ASP:H	1:14:A:ASP:HB2	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	3	0.2
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	3	0.2
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	3	0.2
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	3	0.2
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	3	0.2
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	3	0.2
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	3	0.2
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	3	0.2
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	3	0.2
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	10	0.2
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	10	0.2
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	10	0.2
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	10	0.2
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	10	0.2
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	10	0.2
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	10	0.2
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	10	0.2
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	10	0.2
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	3	0.2
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	3	0.2
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	3	0.2
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	3	0.2
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	3	0.2
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	3	0.2
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	3	0.2
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	3	0.2
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	3	0.2
(4,28)	1:5:A:VAL:HG11	1:6:A:ARG:H	8	0.2
(4,28)	1:5:A:VAL:HG12	1:6:A:ARG:H	8	0.2
(4,28)	1:5:A:VAL:HG13	1:6:A:ARG:H	8	0.2
(3,600)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	8	0.2
(3,600)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	8	0.2
(3,600)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	8	0.2
(3,600)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.2
(3,600)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.2
(3,600)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.2
(3,250)	1:5:A:VAL:HG21	1:6:A:ARG:H	8	0.2
(3,250)	1:5:A:VAL:HG22	1:6:A:ARG:H	8	0.2
(3,250)	1:5:A:VAL:HG23	1:6:A:ARG:H	8	0.2
(3,214)	1:15:A:GLY:HA2	1:16:A:GLY:H	6	0.2
(3,214)	1:15:A:GLY:HA2	1:16:A:GLY:H	10	0.2
(3,195)	1:8:A:TYR:HE1	1:12:A:LEU:HG	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,195)	1:8:A:TYR:HE2	1:12:A:LEU:HG	4	0.2
(3,169)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	8	0.2
(3,1)	1:7:A:LEU:HB3	1:8:A:TYR:H	10	0.2
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	8	0.2
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	8	0.2
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	8	0.2
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.2
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.2
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.2
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	3	0.2
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	3	0.2
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	3	0.2
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	3	0.2
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	3	0.2
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	3	0.2
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	3	0.2
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	3	0.2
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	3	0.2
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	10	0.2
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	10	0.2
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	10	0.2
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	10	0.2
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	10	0.2
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	10	0.2
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	10	0.2
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	10	0.2
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	10	0.2
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	3	0.2
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	3	0.2
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	3	0.2
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	3	0.2
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	3	0.2
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	3	0.2
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	3	0.2
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	3	0.2
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	3	0.2
(2,278)	1:5:A:VAL:HG21	1:6:A:ARG:H	8	0.2
(2,278)	1:5:A:VAL:HG22	1:6:A:ARG:H	8	0.2
(2,278)	1:5:A:VAL:HG23	1:6:A:ARG:H	8	0.2
(2,277)	1:5:A:VAL:HG11	1:6:A:ARG:H	8	0.2
(2,277)	1:5:A:VAL:HG12	1:6:A:ARG:H	8	0.2
(2,277)	1:5:A:VAL:HG13	1:6:A:ARG:H	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,239)	1:15:A:GLY:HA2	1:16:A:GLY:H	6	0.2
(2,239)	1:15:A:GLY:HA2	1:16:A:GLY:H	10	0.2
(2,219)	1:8:A:TYR:HE1	1:12:A:LEU:HG	4	0.2
(2,219)	1:8:A:TYR:HE2	1:12:A:LEU:HG	4	0.2
(2,186)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	8	0.2
(2,1)	1:7:A:LEU:HB3	1:8:A:TYR:H	10	0.2
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG21	9	0.2
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG22	9	0.2
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG23	9	0.2
(1,629)	1:2:A:GLU:HG3	1:5:A:VAL:HB	8	0.2
(1,593)	1:2:A:GLU:HB3	1:6:A:ARG:H	6	0.2
(1,583)	1:6:A:ARG:HB3	1:7:A:LEU:H	1	0.2
(1,570)	1:23:A:PRO:HA	1:24:A:PRO:HD2	5	0.2
(1,531)	1:11:A:TRP:HB3	1:24:A:PRO:HG3	10	0.2
(1,504)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	2	0.2
(1,459)	1:22:A:PRO:HB3	1:22:A:PRO:HG3	10	0.2
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	7	0.2
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	7	0.2
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	2	0.2
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	2	0.2
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	3	0.2
(1,415)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	3	0.2
(1,410)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	1	0.2
(1,410)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	2	0.2
(1,410)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	3	0.2
(1,410)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	4	0.2
(1,410)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	5	0.2
(1,410)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	6	0.2
(1,410)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	7	0.2
(1,410)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	8	0.2
(1,410)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	9	0.2
(1,410)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.2
(1,402)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	8	0.2
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	3	0.2
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	3	0.2
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	3	0.2
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	3	0.2
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	3	0.2
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	3	0.2
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	3	0.2
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	3	0.2
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	6	0.2
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	6	0.2
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	6	0.2
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	6	0.2
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	6	0.2
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	6	0.2
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	6	0.2
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	6	0.2
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	6	0.2
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	10	0.2
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	10	0.2
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	10	0.2
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	10	0.2
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	10	0.2
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	10	0.2
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	10	0.2
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	10	0.2
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	10	0.2
(1,382)	1:12:A:LEU:HD11	1:12:A:LEU:HG	1	0.2
(1,382)	1:12:A:LEU:HD12	1:12:A:LEU:HG	1	0.2
(1,382)	1:12:A:LEU:HD13	1:12:A:LEU:HG	1	0.2
(1,382)	1:12:A:LEU:HD11	1:12:A:LEU:HG	3	0.2
(1,382)	1:12:A:LEU:HD12	1:12:A:LEU:HG	3	0.2
(1,382)	1:12:A:LEU:HD13	1:12:A:LEU:HG	3	0.2
(1,382)	1:12:A:LEU:HD11	1:12:A:LEU:HG	4	0.2
(1,382)	1:12:A:LEU:HD12	1:12:A:LEU:HG	4	0.2
(1,382)	1:12:A:LEU:HD13	1:12:A:LEU:HG	4	0.2
(1,382)	1:12:A:LEU:HD11	1:12:A:LEU:HG	6	0.2
(1,382)	1:12:A:LEU:HD12	1:12:A:LEU:HG	6	0.2
(1,382)	1:12:A:LEU:HD13	1:12:A:LEU:HG	6	0.2
(1,381)	1:12:A:LEU:HD21	1:12:A:LEU:HG	1	0.2
(1,381)	1:12:A:LEU:HD22	1:12:A:LEU:HG	1	0.2
(1,381)	1:12:A:LEU:HD23	1:12:A:LEU:HG	1	0.2
(1,381)	1:12:A:LEU:HD21	1:12:A:LEU:HG	2	0.2
(1,381)	1:12:A:LEU:HD22	1:12:A:LEU:HG	2	0.2
(1,381)	1:12:A:LEU:HD23	1:12:A:LEU:HG	2	0.2
(1,381)	1:12:A:LEU:HD21	1:12:A:LEU:HG	3	0.2
(1,381)	1:12:A:LEU:HD22	1:12:A:LEU:HG	3	0.2
(1,381)	1:12:A:LEU:HD23	1:12:A:LEU:HG	3	0.2
(1,381)	1:12:A:LEU:HD21	1:12:A:LEU:HG	4	0.2
(1,381)	1:12:A:LEU:HD22	1:12:A:LEU:HG	4	0.2
(1,381)	1:12:A:LEU:HD23	1:12:A:LEU:HG	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:12:A:LEU:HD21	1:12:A:LEU:HG	6	0.2
(1,381)	1:12:A:LEU:HD22	1:12:A:LEU:HG	6	0.2
(1,381)	1:12:A:LEU:HD23	1:12:A:LEU:HG	6	0.2
(1,381)	1:12:A:LEU:HD21	1:12:A:LEU:HG	7	0.2
(1,381)	1:12:A:LEU:HD22	1:12:A:LEU:HG	7	0.2
(1,381)	1:12:A:LEU:HD23	1:12:A:LEU:HG	7	0.2
(1,381)	1:12:A:LEU:HD21	1:12:A:LEU:HG	9	0.2
(1,381)	1:12:A:LEU:HD22	1:12:A:LEU:HG	9	0.2
(1,381)	1:12:A:LEU:HD23	1:12:A:LEU:HG	9	0.2
(1,381)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.2
(1,381)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.2
(1,381)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.2
(1,371)	1:11:A:TRP:HA	1:11:A:TRP:HB2	2	0.2
(1,371)	1:11:A:TRP:HA	1:11:A:TRP:HB2	6	0.2
(1,371)	1:11:A:TRP:HA	1:11:A:TRP:HB2	7	0.2
(1,371)	1:11:A:TRP:HA	1:11:A:TRP:HB2	9	0.2
(1,323)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	4	0.2
(1,306)	1:4:A:CYS:HA	1:4:A:CYS:HB2	1	0.2
(1,302)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	2	0.2
(1,302)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	4	0.2
(1,302)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	6	0.2
(1,302)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	8	0.2
(1,203)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	9	0.2
(1,203)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	9	0.2
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	4	0.2
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	4	0.2
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	4	0.2
(1,164)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	3	0.2
(1,164)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	4	0.2
(1,164)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	5	0.2
(1,164)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	6	0.2
(1,164)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	8	0.2
(1,164)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	9	0.2
(1,164)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	0.2
(1,145)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	5	0.2
(1,143)	1:23:A:PRO:HB2	1:25:A:CYS:H	10	0.2
(1,131)	1:9:A:ILE:HA	1:12:A:LEU:H	1	0.2
(1,131)	1:9:A:ILE:HA	1:12:A:LEU:H	6	0.2
(1,87)	1:19:A:SER:H	1:19:A:SER:HG	6	0.2
(1,87)	1:19:A:SER:H	1:19:A:SER:HG	7	0.2
(1,80)	1:5:A:VAL:HA	1:8:A:TYR:H	7	0.2
(1,80)	1:5:A:VAL:HA	1:8:A:TYR:H	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:4:A:CYS:HB3	1:5:A:VAL:H	9	0.2
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	4	0.19
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	4	0.19
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	4	0.19
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	4	0.19
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	4	0.19
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	4	0.19
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	4	0.19
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	4	0.19
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	4	0.19
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	4	0.19
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	4	0.19
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	4	0.19
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	4	0.19
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	4	0.19
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	4	0.19
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	4	0.19
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	4	0.19
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	4	0.19
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	6	0.19
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	6	0.19
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	6	0.19
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	6	0.19
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	6	0.19
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	6	0.19
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	6	0.19
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	6	0.19
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	6	0.19
(4,28)	1:5:A:VAL:HG11	1:6:A:ARG:H	9	0.19
(4,28)	1:5:A:VAL:HG12	1:6:A:ARG:H	9	0.19
(4,28)	1:5:A:VAL:HG13	1:6:A:ARG:H	9	0.19
(4,22)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	3	0.19
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG11	3	0.19
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG12	3	0.19
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG13	3	0.19
(3,600)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	6	0.19
(3,600)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	6	0.19
(3,600)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	6	0.19
(3,587)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	5	0.19
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	7	0.19
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	7	0.19
(3,250)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,250)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	0.19
(3,250)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	0.19
(3,250)	1:5:A:VAL:HG21	1:6:A:ARG:H	9	0.19
(3,250)	1:5:A:VAL:HG22	1:6:A:ARG:H	9	0.19
(3,250)	1:5:A:VAL:HG23	1:6:A:ARG:H	9	0.19
(3,250)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.19
(3,250)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.19
(3,250)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.19
(3,100)	1:6:A:ARG:HB2	1:7:A:LEU:H	7	0.19
(3,1)	1:7:A:LEU:HB3	1:8:A:TYR:H	1	0.19
(3,1)	1:7:A:LEU:HB3	1:8:A:TYR:H	6	0.19
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	6	0.19
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	6	0.19
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	6	0.19
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	4	0.19
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	4	0.19
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	4	0.19
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	4	0.19
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	4	0.19
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	4	0.19
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	4	0.19
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	4	0.19
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	4	0.19
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	4	0.19
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	4	0.19
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	4	0.19
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	4	0.19
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	4	0.19
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	4	0.19
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	4	0.19
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	4	0.19
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	4	0.19
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	6	0.19
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	6	0.19
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	6	0.19
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	6	0.19
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	6	0.19
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	6	0.19
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	6	0.19
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	6	0.19
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	6	0.19
(2,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	7	0.19
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	7	0.19
(2,278)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	0.19
(2,278)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	0.19
(2,278)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	0.19
(2,278)	1:5:A:VAL:HG21	1:6:A:ARG:H	9	0.19
(2,278)	1:5:A:VAL:HG22	1:6:A:ARG:H	9	0.19
(2,278)	1:5:A:VAL:HG23	1:6:A:ARG:H	9	0.19
(2,278)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.19
(2,278)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.19
(2,278)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.19
(2,277)	1:5:A:VAL:HG11	1:6:A:ARG:H	9	0.19
(2,277)	1:5:A:VAL:HG12	1:6:A:ARG:H	9	0.19
(2,277)	1:5:A:VAL:HG13	1:6:A:ARG:H	9	0.19
(2,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	3	0.19
(2,108)	1:6:A:ARG:HB2	1:7:A:LEU:H	7	0.19
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG11	3	0.19
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG12	3	0.19
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG13	3	0.19
(2,1)	1:7:A:LEU:HB3	1:8:A:TYR:H	1	0.19
(2,1)	1:7:A:LEU:HB3	1:8:A:TYR:H	6	0.19
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	10	0.19
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	10	0.19
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	10	0.19
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	10	0.19
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	10	0.19
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	10	0.19
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	10	0.19
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	10	0.19
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	10	0.19
(1,629)	1:2:A:GLU:HG3	1:5:A:VAL:HB	2	0.19
(1,599)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	9	0.19
(1,599)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	9	0.19
(1,570)	1:23:A:PRO:HA	1:24:A:PRO:HD2	6	0.19
(1,570)	1:23:A:PRO:HA	1:24:A:PRO:HD2	8	0.19
(1,569)	1:23:A:PRO:HA	1:24:A:PRO:HD3	1	0.19
(1,569)	1:23:A:PRO:HA	1:24:A:PRO:HD3	4	0.19
(1,558)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	2	0.19
(1,540)	1:7:A:LEU:HA	1:10:A:GLN:HB2	4	0.19
(1,516)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	5	0.19
(1,516)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	7	0.19
(1,516)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	9	0.19
(1,504)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	1	0.19
(1,504)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	3	0.19
(1,504)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	4	0.19
(1,504)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	5	0.19
(1,504)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	6	0.19
(1,504)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	7	0.19
(1,504)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	8	0.19
(1,504)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	9	0.19
(1,504)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	10	0.19
(1,469)	1:23:A:PRO:HA	1:23:A:PRO:HD3	5	0.19
(1,469)	1:23:A:PRO:HA	1:23:A:PRO:HD3	6	0.19
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	6	0.19
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	6	0.19
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	10	0.19
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	10	0.19
(1,420)	1:18:A:SER:HA	1:18:A:SER:HB2	3	0.19
(1,402)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	1	0.19
(1,402)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	2	0.19
(1,402)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	3	0.19
(1,402)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	4	0.19
(1,402)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	5	0.19
(1,402)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	6	0.19
(1,402)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	7	0.19
(1,402)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	9	0.19
(1,402)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	10	0.19
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	8	0.19
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	8	0.19
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	8	0.19
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	8	0.19
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	8	0.19
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	8	0.19
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	8	0.19
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	8	0.19
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	8	0.19
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	9	0.19
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	9	0.19
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	9	0.19
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	9	0.19
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	9	0.19
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	9	0.19
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	9	0.19
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	9	0.19
(1,381)	1:12:A:LEU:HD21	1:12:A:LEU:HG	5	0.19
(1,381)	1:12:A:LEU:HD22	1:12:A:LEU:HG	5	0.19
(1,381)	1:12:A:LEU:HD23	1:12:A:LEU:HG	5	0.19
(1,371)	1:11:A:TRP:HA	1:11:A:TRP:HB2	1	0.19
(1,371)	1:11:A:TRP:HA	1:11:A:TRP:HB2	3	0.19
(1,371)	1:11:A:TRP:HA	1:11:A:TRP:HB2	8	0.19
(1,362)	1:10:A:GLN:HA	1:10:A:GLN:HB2	3	0.19
(1,334)	1:7:A:LEU:HA	1:7:A:LEU:HB2	6	0.19
(1,323)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	9	0.19
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG21	7	0.19
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG22	7	0.19
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG23	7	0.19
(1,308)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	5	0.19
(1,308)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	9	0.19
(1,306)	1:4:A:CYS:HA	1:4:A:CYS:HB2	8	0.19
(1,306)	1:4:A:CYS:HA	1:4:A:CYS:HB2	10	0.19
(1,304)	1:3:A:GLU:HA	1:3:A:GLU:HB2	1	0.19
(1,304)	1:3:A:GLU:HA	1:3:A:GLU:HB3	1	0.19
(1,302)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	1	0.19
(1,302)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	3	0.19
(1,302)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	5	0.19
(1,302)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	7	0.19
(1,302)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	9	0.19
(1,302)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	10	0.19
(1,222)	1:8:A:TYR:HE1	1:9:A:ILE:HG12	6	0.19
(1,222)	1:8:A:TYR:HE2	1:9:A:ILE:HG12	6	0.19
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	4	0.19
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	4	0.19
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	4	0.19
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	4	0.19
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	4	0.19
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	4	0.19
(1,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	3	0.19
(1,164)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	1	0.19
(1,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	3	0.19
(1,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	3	0.19
(1,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	9	0.19
(1,138)	1:8:A:TYR:HB2	1:9:A:ILE:H	7	0.19
(1,138)	1:8:A:TYR:HB3	1:9:A:ILE:H	7	0.19
(1,80)	1:5:A:VAL:HA	1:8:A:TYR:H	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:14:A:ASP:H	1:14:A:ASP:HB2	10	0.19
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	1	0.18
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	1	0.18
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	1	0.18
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	1	0.18
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	1	0.18
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	1	0.18
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	1	0.18
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	1	0.18
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	1	0.18
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	5	0.18
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	5	0.18
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	5	0.18
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	5	0.18
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	5	0.18
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	5	0.18
(4,27)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.18
(4,27)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.18
(3,600)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	4	0.18
(3,600)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	4	0.18
(3,600)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	4	0.18
(3,587)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	7	0.18
(3,572)	1:17:A:PRO:HB2	1:18:A:SER:HB2	10	0.18
(3,427)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	4	0.18
(3,427)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	6	0.18
(3,427)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	9	0.18
(3,427)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	10	0.18
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	6	0.18
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	6	0.18
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	10	0.18
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.18
(3,141)	1:11:A:TRP:HD1	1:19:A:SER:HB3	7	0.18
(3,99)	1:9:A:ILE:H	1:9:A:ILE:HG12	2	0.18
(3,22)	1:3:A:GLU:H	1:3:A:GLU:HG2	1	0.18
(3,22)	1:3:A:GLU:H	1:3:A:GLU:HG3	1	0.18
(3,21)	1:2:A:GLU:HB2	1:3:A:GLU:H	10	0.18
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	4	0.18
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	4	0.18
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	4	0.18
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	1	0.18
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	1	0.18
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	1	0.18
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	1	0.18
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	1	0.18
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	1	0.18
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	1	0.18
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	1	0.18
(2,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	7	0.18
(2,616)	1:17:A:PRO:HB2	1:18:A:SER:HB2	10	0.18
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	5	0.18
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	5	0.18
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	5	0.18
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	5	0.18
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	5	0.18
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	5	0.18
(2,461)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	4	0.18
(2,461)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	6	0.18
(2,461)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	9	0.18
(2,461)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	10	0.18
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	6	0.18
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	6	0.18
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	10	0.18
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.18
(2,273)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.18
(2,273)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.18
(2,152)	1:11:A:TRP:HD1	1:19:A:SER:HB3	7	0.18
(2,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	2	0.18
(2,26)	1:3:A:GLU:H	1:3:A:GLU:HG2	1	0.18
(2,26)	1:3:A:GLU:H	1:3:A:GLU:HG3	1	0.18
(2,25)	1:2:A:GLU:HB2	1:3:A:GLU:H	10	0.18
(1,672)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	1	0.18
(1,672)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	2	0.18
(1,672)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	3	0.18
(1,672)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	6	0.18
(1,672)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	7	0.18
(1,672)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	9	0.18
(1,672)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	10	0.18
(1,665)	1:10:A:GLN:HA	1:13:A:LYS:HD3	2	0.18
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG21	8	0.18
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG22	8	0.18
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG23	8	0.18
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	6	0.18
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	6	0.18
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	6	0.18
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	6	0.18
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	6	0.18
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	6	0.18
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	6	0.18
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	6	0.18
(1,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	5	0.18
(1,612)	1:15:A:GLY:HA3	1:19:A:SER:HB2	5	0.18
(1,593)	1:2:A:GLU:HB3	1:6:A:ARG:H	10	0.18
(1,583)	1:6:A:ARG:HB3	1:7:A:LEU:H	2	0.18
(1,576)	1:10:A:GLN:H	1:12:A:LEU:H	2	0.18
(1,569)	1:23:A:PRO:HA	1:24:A:PRO:HD3	5	0.18
(1,564)	1:11:A:TRP:HA	1:14:A:ASP:HB2	10	0.18
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	5	0.18
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	5	0.18
(1,560)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	5	0.18
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	5	0.18
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	5	0.18
(1,560)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	5	0.18
(1,552)	1:22:A:PRO:HA	1:23:A:PRO:HD3	1	0.18
(1,516)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	1	0.18
(1,516)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	2	0.18
(1,516)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	3	0.18
(1,516)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	4	0.18
(1,516)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	6	0.18
(1,516)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	10	0.18
(1,469)	1:23:A:PRO:HA	1:23:A:PRO:HD3	10	0.18
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	4	0.18
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	4	0.18
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	4	0.18
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	4	0.18
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	4	0.18
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	4	0.18
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	4	0.18
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	4	0.18
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	4	0.18
(1,371)	1:11:A:TRP:HA	1:11:A:TRP:HB2	10	0.18
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB2	1	0.18
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB3	1	0.18
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB2	10	0.18
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB3	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	5	0.18
(1,341)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	7	0.18
(1,341)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	8	0.18
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG11	4	0.18
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG12	4	0.18
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG13	4	0.18
(1,308)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	1	0.18
(1,308)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	2	0.18
(1,308)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	3	0.18
(1,308)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	4	0.18
(1,308)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	6	0.18
(1,308)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	7	0.18
(1,308)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	8	0.18
(1,308)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	10	0.18
(1,297)	1:2:A:GLU:HA	1:2:A:GLU:HG2	5	0.18
(1,206)	1:23:A:PRO:HB3	1:25:A:CYS:H	10	0.18
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.18
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.18
(1,193)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.18
(1,184)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	8	0.18
(1,184)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	8	0.18
(1,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	4	0.18
(1,150)	1:8:A:TYR:HD1	1:9:A:ILE:HA	2	0.18
(1,150)	1:8:A:TYR:HD2	1:9:A:ILE:HA	2	0.18
(1,145)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	6	0.18
(1,105)	1:7:A:LEU:H	1:7:A:LEU:HG	9	0.18
(1,71)	1:25:A:CYS:H	1:25:A:CYS:HB3	9	0.18
(1,11)	1:16:A:GLY:H	1:16:A:GLY:HA2	4	0.18
(1,11)	1:16:A:GLY:H	1:16:A:GLY:HA2	6	0.18
(1,11)	1:16:A:GLY:H	1:16:A:GLY:HA2	10	0.18
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	1	0.17
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	1	0.17
(4,51)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	1	0.17
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	1	0.17
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	1	0.17
(4,51)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	1	0.17
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	1	0.17
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	1	0.17
(4,51)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	1	0.17
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	10	0.17
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	10	0.17
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	10	0.17
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	10	0.17
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	10	0.17
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	10	0.17
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	10	0.17
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	10	0.17
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	8	0.17
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	8	0.17
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	8	0.17
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	9	0.17
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	9	0.17
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	9	0.17
(4,27)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.17
(4,27)	1:12:A:LEU:H	1:12:A:LEU:HB3	5	0.17
(4,27)	1:12:A:LEU:H	1:12:A:LEU:HB3	8	0.17
(4,27)	1:12:A:LEU:H	1:12:A:LEU:HB3	9	0.17
(4,27)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.17
(4,3)	1:12:A:LEU:HD21	1:13:A:LYS:H	8	0.17
(4,3)	1:12:A:LEU:HD22	1:13:A:LYS:H	8	0.17
(4,3)	1:12:A:LEU:HD23	1:13:A:LYS:H	8	0.17
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG11	5	0.17
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG12	5	0.17
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG13	5	0.17
(3,587)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	3	0.17
(3,572)	1:17:A:PRO:HB2	1:18:A:SER:HB2	3	0.17
(3,427)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	5	0.17
(3,427)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	7	0.17
(3,375)	1:17:A:PRO:HA	1:17:A:PRO:HG2	2	0.17
(3,241)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	7	0.17
(3,231)	1:10:A:GLN:HG2	1:11:A:TRP:H	9	0.17
(3,198)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	8	0.17
(3,198)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	8	0.17
(3,189)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	4	0.17
(3,169)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	9	0.17
(3,24)	1:4:A:CYS:H	1:4:A:CYS:HB2	5	0.17
(3,1)	1:7:A:LEU:HB3	1:8:A:TYR:H	9	0.17
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD21	1	0.17
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD22	1	0.17
(2,645)	1:9:A:ILE:HD11	1:12:A:LEU:HD23	1	0.17
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD21	1	0.17
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD22	1	0.17
(2,645)	1:9:A:ILE:HD12	1:12:A:LEU:HD23	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD21	1	0.17
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD22	1	0.17
(2,645)	1:9:A:ILE:HD13	1:12:A:LEU:HD23	1	0.17
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	10	0.17
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	10	0.17
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	10	0.17
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	10	0.17
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	10	0.17
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	10	0.17
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	10	0.17
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	10	0.17
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	10	0.17
(2,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	3	0.17
(2,616)	1:17:A:PRO:HB2	1:18:A:SER:HB2	3	0.17
(2,461)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	5	0.17
(2,461)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	7	0.17
(2,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	2	0.17
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	8	0.17
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	8	0.17
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	8	0.17
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	9	0.17
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	9	0.17
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	9	0.17
(2,273)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.17
(2,273)	1:12:A:LEU:H	1:12:A:LEU:HB3	5	0.17
(2,273)	1:12:A:LEU:H	1:12:A:LEU:HB3	8	0.17
(2,273)	1:12:A:LEU:H	1:12:A:LEU:HB3	9	0.17
(2,273)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.17
(2,266)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	7	0.17
(2,256)	1:10:A:GLN:HG2	1:11:A:TRP:H	9	0.17
(2,223)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	8	0.17
(2,223)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	8	0.17
(2,211)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	4	0.17
(2,186)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	9	0.17
(2,28)	1:4:A:CYS:H	1:4:A:CYS:HB2	5	0.17
(2,12)	1:12:A:LEU:HD21	1:13:A:LYS:H	8	0.17
(2,12)	1:12:A:LEU:HD22	1:13:A:LYS:H	8	0.17
(2,12)	1:12:A:LEU:HD23	1:13:A:LYS:H	8	0.17
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG11	5	0.17
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG12	5	0.17
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG13	5	0.17
(2,1)	1:7:A:LEU:HB3	1:8:A:TYR:H	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	4	0.17
(1,672)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	5	0.17
(1,672)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	8	0.17
(1,664)	1:10:A:GLN:HA	1:13:A:LYS:HD2	6	0.17
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB2	4	0.17
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB3	4	0.17
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB2	8	0.17
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB3	8	0.17
(1,612)	1:15:A:GLY:HA3	1:19:A:SER:HB2	1	0.17
(1,612)	1:15:A:GLY:HA3	1:19:A:SER:HB2	2	0.17
(1,612)	1:15:A:GLY:HA3	1:19:A:SER:HB2	6	0.17
(1,612)	1:15:A:GLY:HA3	1:19:A:SER:HB2	7	0.17
(1,570)	1:23:A:PRO:HA	1:24:A:PRO:HD2	4	0.17
(1,540)	1:7:A:LEU:HA	1:10:A:GLN:HB2	5	0.17
(1,534)	1:21:A:ARG:HB3	1:22:A:PRO:HD2	7	0.17
(1,471)	1:11:A:TRP:HH2	1:23:A:PRO:HD3	5	0.17
(1,448)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	5	0.17
(1,448)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	9	0.17
(1,420)	1:18:A:SER:HA	1:18:A:SER:HB2	6	0.17
(1,382)	1:12:A:LEU:HD11	1:12:A:LEU:HG	5	0.17
(1,382)	1:12:A:LEU:HD12	1:12:A:LEU:HG	5	0.17
(1,382)	1:12:A:LEU:HD13	1:12:A:LEU:HG	5	0.17
(1,371)	1:11:A:TRP:HA	1:11:A:TRP:HB2	4	0.17
(1,371)	1:11:A:TRP:HA	1:11:A:TRP:HB2	5	0.17
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB2	4	0.17
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB3	4	0.17
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB2	9	0.17
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB3	9	0.17
(1,341)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	2	0.17
(1,341)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	3	0.17
(1,341)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	4	0.17
(1,341)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	6	0.17
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG21	2	0.17
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG22	2	0.17
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG23	2	0.17
(1,306)	1:4:A:CYS:HA	1:4:A:CYS:HB2	5	0.17
(1,297)	1:2:A:GLU:HA	1:2:A:GLU:HG2	3	0.17
(1,268)	1:8:A:TYR:H	1:24:A:PRO:HG2	1	0.17
(1,222)	1:8:A:TYR:HE1	1:9:A:ILE:HG12	9	0.17
(1,222)	1:8:A:TYR:HE2	1:9:A:ILE:HG12	9	0.17
(1,131)	1:9:A:ILE:HA	1:12:A:LEU:H	3	0.17
(1,131)	1:9:A:ILE:HA	1:12:A:LEU:H	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:19:A:SER:H	1:19:A:SER:HG	8	0.17
(1,75)	1:19:A:SER:H	1:19:A:SER:HB3	2	0.17
(1,71)	1:25:A:CYS:H	1:25:A:CYS:HB3	2	0.17
(1,61)	1:20:A:GLY:H	1:20:A:GLY:HA3	8	0.17
(1,41)	1:14:A:ASP:H	1:14:A:ASP:HB2	3	0.17
(1,11)	1:16:A:GLY:H	1:16:A:GLY:HA2	1	0.17
(1,11)	1:16:A:GLY:H	1:16:A:GLY:HA2	2	0.17
(1,11)	1:16:A:GLY:H	1:16:A:GLY:HA2	3	0.17
(1,11)	1:16:A:GLY:H	1:16:A:GLY:HA2	5	0.17
(1,11)	1:16:A:GLY:H	1:16:A:GLY:HA2	9	0.17
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD11	8	0.16
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD12	8	0.16
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD13	8	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	1	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	1	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	1	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	3	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	3	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	3	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	5	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	5	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	5	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	6	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	6	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	6	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	10	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	10	0.16
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	10	0.16
(4,4)	1:9:A:ILE:HG21	1:10:A:GLN:H	2	0.16
(4,4)	1:9:A:ILE:HG22	1:10:A:GLN:H	2	0.16
(4,4)	1:9:A:ILE:HG23	1:10:A:GLN:H	2	0.16
(3,613)	1:10:A:GLN:HA	1:13:A:LYS:HD2	1	0.16
(3,587)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	8	0.16
(3,540)	1:5:A:VAL:HG21	1:9:A:ILE:H	3	0.16
(3,540)	1:5:A:VAL:HG22	1:9:A:ILE:H	3	0.16
(3,540)	1:5:A:VAL:HG23	1:9:A:ILE:H	3	0.16
(3,427)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	8	0.16
(3,375)	1:17:A:PRO:HA	1:17:A:PRO:HG2	1	0.16
(3,375)	1:17:A:PRO:HA	1:17:A:PRO:HG2	6	0.16
(3,169)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	10	0.16
(3,98)	1:6:A:ARG:HG3	1:7:A:LEU:H	2	0.16
(3,98)	1:6:A:ARG:HG3	1:7:A:LEU:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,664)	1:10:A:GLN:HA	1:13:A:LYS:HD2	1	0.16
(2,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	8	0.16
(2,581)	1:5:A:VAL:HG21	1:9:A:ILE:H	3	0.16
(2,581)	1:5:A:VAL:HG22	1:9:A:ILE:H	3	0.16
(2,581)	1:5:A:VAL:HG23	1:9:A:ILE:H	3	0.16
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	8	0.16
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	8	0.16
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	8	0.16
(2,461)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	8	0.16
(2,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	1	0.16
(2,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	6	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	1	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	1	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	1	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	3	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	3	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	3	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	5	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	5	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	5	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	6	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	6	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	6	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	10	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	10	0.16
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	10	0.16
(2,186)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	10	0.16
(2,106)	1:6:A:ARG:HG3	1:7:A:LEU:H	2	0.16
(2,106)	1:6:A:ARG:HG3	1:7:A:LEU:H	8	0.16
(2,15)	1:9:A:ILE:HG21	1:10:A:GLN:H	2	0.16
(2,15)	1:9:A:ILE:HG22	1:10:A:GLN:H	2	0.16
(2,15)	1:9:A:ILE:HG23	1:10:A:GLN:H	2	0.16
(1,668)	1:1:A:GLU:HA	1:1:A:GLU:HB3	1	0.16
(1,629)	1:2:A:GLU:HG3	1:5:A:VAL:HB	10	0.16
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB2	6	0.16
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB3	6	0.16
(1,570)	1:23:A:PRO:HA	1:24:A:PRO:HD2	7	0.16
(1,569)	1:23:A:PRO:HA	1:24:A:PRO:HD3	7	0.16
(1,569)	1:23:A:PRO:HA	1:24:A:PRO:HD3	8	0.16
(1,528)	1:11:A:TRP:HB3	1:24:A:PRO:HD3	2	0.16
(1,506)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	2	0.16
(1,495)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	2	0.16
(1,495)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	3	0.16
(1,495)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	4	0.16
(1,495)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	5	0.16
(1,495)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	6	0.16
(1,495)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	7	0.16
(1,495)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	8	0.16
(1,495)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	9	0.16
(1,495)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	10	0.16
(1,448)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	1	0.16
(1,448)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	2	0.16
(1,448)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	3	0.16
(1,448)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	4	0.16
(1,448)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	6	0.16
(1,448)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	7	0.16
(1,448)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	8	0.16
(1,448)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	10	0.16
(1,420)	1:18:A:SER:HA	1:18:A:SER:HB2	10	0.16
(1,400)	1:14:A:ASP:HA	1:14:A:ASP:HB2	8	0.16
(1,385)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	8	0.16
(1,385)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	8	0.16
(1,385)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	8	0.16
(1,366)	1:10:A:GLN:HB3	1:10:A:GLN:HG3	8	0.16
(1,360)	1:10:A:GLN:HA	1:10:A:GLN:HG3	3	0.16
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB2	3	0.16
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB3	3	0.16
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB2	6	0.16
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB3	6	0.16
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB2	7	0.16
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB3	7	0.16
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB2	8	0.16
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB3	8	0.16
(1,341)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	1	0.16
(1,341)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	9	0.16
(1,341)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.16
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG11	6	0.16
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG12	6	0.16
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG13	6	0.16
(1,306)	1:4:A:CYS:HA	1:4:A:CYS:HB2	7	0.16
(1,268)	1:8:A:TYR:H	1:24:A:PRO:HG2	10	0.16
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	5	0.16
(1,220)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	1	0.16
(1,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	9	0.16
(1,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	7	0.16
(1,150)	1:8:A:TYR:HD1	1:9:A:ILE:HA	7	0.16
(1,150)	1:8:A:TYR:HD2	1:9:A:ILE:HA	7	0.16
(1,127)	1:20:A:GLY:HA3	1:21:A:ARG:H	7	0.16
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	9	0.16
(1,102)	1:10:A:GLN:HB3	1:11:A:TRP:H	8	0.16
(1,61)	1:20:A:GLY:H	1:20:A:GLY:HA3	1	0.16
(1,11)	1:16:A:GLY:H	1:16:A:GLY:HA2	7	0.16
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	8	0.15
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	8	0.15
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	8	0.15
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	8	0.15
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	8	0.15
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	8	0.15
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	8	0.15
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	8	0.15
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	8	0.15
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	2	0.15
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	2	0.15
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	2	0.15
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	2	0.15
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	2	0.15
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	2	0.15
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	7	0.15
(4,44)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	7	0.15
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	7	0.15
(4,44)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	7	0.15
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	7	0.15
(4,44)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	7	0.15
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD11	9	0.15
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD12	9	0.15
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD13	9	0.15
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	4	0.15
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	4	0.15
(4,33)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	4	0.15
(4,22)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	9	0.15
(4,5)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.15
(3,587)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	2	0.15
(3,587)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	4	0.15
(3,540)	1:5:A:VAL:HG21	1:9:A:ILE:H	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,540)	1:5:A:VAL:HG22	1:9:A:ILE:H	4	0.15
(3,540)	1:5:A:VAL:HG23	1:9:A:ILE:H	4	0.15
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	1	0.15
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	1	0.15
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	2	0.15
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	2	0.15
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	3	0.15
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	3	0.15
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	5	0.15
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	5	0.15
(3,375)	1:17:A:PRO:HA	1:17:A:PRO:HG2	8	0.15
(3,195)	1:8:A:TYR:HE1	1:12:A:LEU:HG	8	0.15
(3,195)	1:8:A:TYR:HE2	1:12:A:LEU:HG	8	0.15
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	3	0.15
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	3	0.15
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	3	0.15
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	3	0.15
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	3	0.15
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	3	0.15
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	6	0.15
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	6	0.15
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	6	0.15
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	6	0.15
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	6	0.15
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	6	0.15
(3,169)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	1	0.15
(3,169)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	5	0.15
(3,169)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	6	0.15
(3,169)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	7	0.15
(3,103)	1:7:A:LEU:H	1:10:A:GLN:HB3	1	0.15
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	8	0.15
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	8	0.15
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	8	0.15
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	8	0.15
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	8	0.15
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	8	0.15
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	8	0.15
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	8	0.15
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	8	0.15
(2,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	2	0.15
(2,632)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	4	0.15
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	2	0.15
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	2	0.15
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	2	0.15
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	2	0.15
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	2	0.15
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	7	0.15
(2,607)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	7	0.15
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	7	0.15
(2,607)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	7	0.15
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	7	0.15
(2,607)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	7	0.15
(2,581)	1:5:A:VAL:HG21	1:9:A:ILE:H	4	0.15
(2,581)	1:5:A:VAL:HG22	1:9:A:ILE:H	4	0.15
(2,581)	1:5:A:VAL:HG23	1:9:A:ILE:H	4	0.15
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	9	0.15
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	9	0.15
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	9	0.15
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	1	0.15
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	1	0.15
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	2	0.15
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	2	0.15
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	3	0.15
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	3	0.15
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	5	0.15
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	5	0.15
(2,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	8	0.15
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	4	0.15
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	4	0.15
(2,386)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	4	0.15
(2,219)	1:8:A:TYR:HE1	1:12:A:LEU:HG	8	0.15
(2,219)	1:8:A:TYR:HE2	1:12:A:LEU:HG	8	0.15
(2,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	9	0.15
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	3	0.15
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	3	0.15
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	3	0.15
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	3	0.15
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	3	0.15
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	3	0.15
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	6	0.15
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	6	0.15
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	6	0.15
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	6	0.15
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	6	0.15
(2,186)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	1	0.15
(2,186)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	5	0.15
(2,186)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	6	0.15
(2,186)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	7	0.15
(2,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	1	0.15
(2,31)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.15
(1,612)	1:15:A:GLY:HA3	1:19:A:SER:HB2	3	0.15
(1,612)	1:15:A:GLY:HA3	1:19:A:SER:HB2	10	0.15
(1,592)	1:2:A:GLU:HB2	1:6:A:ARG:H	1	0.15
(1,590)	1:24:A:PRO:HB2	1:25:A:CYS:H	3	0.15
(1,569)	1:23:A:PRO:HA	1:24:A:PRO:HD3	3	0.15
(1,540)	1:7:A:LEU:HA	1:10:A:GLN:HB2	10	0.15
(1,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	1	0.15
(1,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	0.15
(1,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	0.15
(1,506)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	4	0.15
(1,506)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	5	0.15
(1,506)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	6	0.15
(1,485)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	2	0.15
(1,469)	1:23:A:PRO:HA	1:23:A:PRO:HD3	2	0.15
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	1	0.15
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	1	0.15
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	3	0.15
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	3	0.15
(1,439)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	1	0.15
(1,439)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	2	0.15
(1,439)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	4	0.15
(1,439)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	5	0.15
(1,439)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	6	0.15
(1,439)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	7	0.15
(1,439)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	8	0.15
(1,439)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	10	0.15
(1,385)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	9	0.15
(1,385)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	9	0.15
(1,385)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	9	0.15
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	2	0.15
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	2	0.15
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	2	0.15
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB2	2	0.15
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB3	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB2	5	0.15
(1,344)	1:8:A:TYR:HA	1:8:A:TYR:HB3	5	0.15
(1,316)	1:6:A:ARG:HA	1:6:A:ARG:HB2	7	0.15
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG11	1	0.15
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG12	1	0.15
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG13	1	0.15
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG11	10	0.15
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG12	10	0.15
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG13	10	0.15
(1,258)	1:14:A:ASP:HB3	1:16:A:GLY:H	4	0.15
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	5	0.15
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	5	0.15
(1,191)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	5	0.15
(1,160)	1:11:A:TRP:HZ3	1:17:A:PRO:HD2	8	0.15
(1,145)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	1	0.15
(1,138)	1:8:A:TYR:HB2	1:9:A:ILE:H	2	0.15
(1,138)	1:8:A:TYR:HB3	1:9:A:ILE:H	2	0.15
(1,131)	1:9:A:ILE:HA	1:12:A:LEU:H	10	0.15
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.15
(1,86)	1:18:A:SER:HA	1:19:A:SER:H	2	0.15
(1,26)	1:3:A:GLU:H	1:3:A:GLU:HG2	3	0.15
(1,26)	1:3:A:GLU:H	1:3:A:GLU:HG3	3	0.15
(1,2)	1:11:A:TRP:HE1	1:16:A:GLY:HA3	8	0.15
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	9	0.14
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	9	0.14
(4,49)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	9	0.14
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	9	0.14
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	9	0.14
(4,49)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	9	0.14
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	9	0.14
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	9	0.14
(4,49)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	9	0.14
(4,27)	1:12:A:LEU:H	1:12:A:LEU:HB3	1	0.14
(4,22)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	5	0.14
(4,22)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	8	0.14
(4,4)	1:9:A:ILE:HG21	1:10:A:GLN:H	7	0.14
(4,4)	1:9:A:ILE:HG22	1:10:A:GLN:H	7	0.14
(4,4)	1:9:A:ILE:HG23	1:10:A:GLN:H	7	0.14
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	5	0.14
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	5	0.14
(3,593)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	5	0.14
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	4	0.14
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	8	0.14
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	8	0.14
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	9	0.14
(3,406)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	9	0.14
(3,250)	1:5:A:VAL:HG21	1:6:A:ARG:H	3	0.14
(3,250)	1:5:A:VAL:HG22	1:6:A:ARG:H	3	0.14
(3,250)	1:5:A:VAL:HG23	1:6:A:ARG:H	3	0.14
(3,241)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	6	0.14
(3,241)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	10	0.14
(3,198)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	2	0.14
(3,198)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	2	0.14
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.14
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.14
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.14
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.14
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.14
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.14
(3,169)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	3	0.14
(3,108)	1:24:A:PRO:HG3	1:25:A:CYS:H	2	0.14
(3,27)	1:10:A:GLN:H	1:10:A:GLN:HB3	4	0.14
(3,22)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.14
(3,22)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.14
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD11	9	0.14
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD12	9	0.14
(2,642)	1:9:A:ILE:HG21	1:12:A:LEU:HD13	9	0.14
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD11	9	0.14
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD12	9	0.14
(2,642)	1:9:A:ILE:HG22	1:12:A:LEU:HD13	9	0.14
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD11	9	0.14
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD12	9	0.14
(2,642)	1:9:A:ILE:HG23	1:12:A:LEU:HD13	9	0.14
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD11	5	0.14
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD12	5	0.14
(2,638)	1:9:A:ILE:HG13	1:12:A:LEU:HD13	5	0.14
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	4	0.14
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	4	0.14
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	8	0.14
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	8	0.14
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	9	0.14
(2,440)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	9	0.14
(2,278)	1:5:A:VAL:HG21	1:6:A:ARG:H	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,278)	1:5:A:VAL:HG22	1:6:A:ARG:H	3	0.14
(2,278)	1:5:A:VAL:HG23	1:6:A:ARG:H	3	0.14
(2,273)	1:12:A:LEU:H	1:12:A:LEU:HB3	1	0.14
(2,266)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	6	0.14
(2,266)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	10	0.14
(2,223)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	2	0.14
(2,223)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	2	0.14
(2,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	5	0.14
(2,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	8	0.14
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.14
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.14
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.14
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.14
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.14
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.14
(2,186)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	3	0.14
(2,117)	1:24:A:PRO:HG3	1:25:A:CYS:H	2	0.14
(2,32)	1:10:A:GLN:H	1:10:A:GLN:HB3	4	0.14
(2,26)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.14
(2,26)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.14
(2,15)	1:9:A:ILE:HG21	1:10:A:GLN:H	7	0.14
(2,15)	1:9:A:ILE:HG22	1:10:A:GLN:H	7	0.14
(2,15)	1:9:A:ILE:HG23	1:10:A:GLN:H	7	0.14
(1,633)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	2	0.14
(1,612)	1:15:A:GLY:HA3	1:19:A:SER:HB2	4	0.14
(1,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	9	0.14
(1,590)	1:24:A:PRO:HB2	1:25:A:CYS:H	6	0.14
(1,589)	1:23:A:PRO:HA	1:25:A:CYS:H	2	0.14
(1,570)	1:23:A:PRO:HA	1:24:A:PRO:HD2	3	0.14
(1,570)	1:23:A:PRO:HA	1:24:A:PRO:HD2	10	0.14
(1,569)	1:23:A:PRO:HA	1:24:A:PRO:HD3	6	0.14
(1,569)	1:23:A:PRO:HA	1:24:A:PRO:HD3	10	0.14
(1,564)	1:11:A:TRP:HA	1:14:A:ASP:HB2	8	0.14
(1,551)	1:22:A:PRO:HA	1:23:A:PRO:HD2	2	0.14
(1,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	0.14
(1,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	0.14
(1,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	0.14
(1,512)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	2	0.14
(1,506)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	1	0.14
(1,506)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	3	0.14
(1,506)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	7	0.14
(1,506)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,506)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	9	0.14
(1,506)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	10	0.14
(1,505)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	9	0.14
(1,505)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	10	0.14
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	2	0.14
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	2	0.14
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	5	0.14
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	5	0.14
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	8	0.14
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	8	0.14
(1,439)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	3	0.14
(1,439)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	9	0.14
(1,370)	1:11:A:TRP:HA	1:11:A:TRP:HB3	1	0.14
(1,370)	1:11:A:TRP:HA	1:11:A:TRP:HB3	2	0.14
(1,370)	1:11:A:TRP:HA	1:11:A:TRP:HB3	3	0.14
(1,370)	1:11:A:TRP:HA	1:11:A:TRP:HB3	4	0.14
(1,370)	1:11:A:TRP:HA	1:11:A:TRP:HB3	5	0.14
(1,370)	1:11:A:TRP:HA	1:11:A:TRP:HB3	6	0.14
(1,370)	1:11:A:TRP:HA	1:11:A:TRP:HB3	7	0.14
(1,370)	1:11:A:TRP:HA	1:11:A:TRP:HB3	8	0.14
(1,370)	1:11:A:TRP:HA	1:11:A:TRP:HB3	9	0.14
(1,370)	1:11:A:TRP:HA	1:11:A:TRP:HB3	10	0.14
(1,366)	1:10:A:GLN:HB3	1:10:A:GLN:HG3	6	0.14
(1,366)	1:10:A:GLN:HB3	1:10:A:GLN:HG3	9	0.14
(1,366)	1:10:A:GLN:HB3	1:10:A:GLN:HG3	10	0.14
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG11	8	0.14
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG12	8	0.14
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG13	8	0.14
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG21	5	0.14
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG22	5	0.14
(1,310)	1:5:A:VAL:HA	1:5:A:VAL:HG23	5	0.14
(1,222)	1:8:A:TYR:HE1	1:9:A:ILE:HG12	3	0.14
(1,222)	1:8:A:TYR:HE2	1:9:A:ILE:HG12	3	0.14
(1,204)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	2	0.14
(1,204)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	2	0.14
(1,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	6	0.14
(1,157)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	1	0.14
(1,145)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	2	0.14
(1,145)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	4	0.14
(1,109)	1:12:A:LEU:H	1:12:A:LEU:HB2	1	0.14
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	4	0.14
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:19:A:SER:H	1:19:A:SER:HG	3	0.14
(1,33)	1:10:A:GLN:H	1:10:A:GLN:HB2	3	0.14
(1,28)	1:4:A:CYS:H	1:4:A:CYS:HB2	8	0.14
(1,27)	1:4:A:CYS:H	1:4:A:CYS:HB3	9	0.14
(1,11)	1:16:A:GLY:H	1:16:A:GLY:HA2	8	0.14
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	2	0.13
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	2	0.13
(4,48)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	2	0.13
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	2	0.13
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	2	0.13
(4,48)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	2	0.13
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	2	0.13
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	2	0.13
(4,48)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	2	0.13
(4,32)	1:9:A:ILE:HB	1:9:A:ILE:HG13	5	0.13
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG11	2	0.13
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG12	2	0.13
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG13	2	0.13
(3,540)	1:5:A:VAL:HG21	1:9:A:ILE:H	1	0.13
(3,540)	1:5:A:VAL:HG22	1:9:A:ILE:H	1	0.13
(3,540)	1:5:A:VAL:HG23	1:9:A:ILE:H	1	0.13
(3,540)	1:5:A:VAL:HG21	1:9:A:ILE:H	6	0.13
(3,540)	1:5:A:VAL:HG22	1:9:A:ILE:H	6	0.13
(3,540)	1:5:A:VAL:HG23	1:9:A:ILE:H	6	0.13
(3,540)	1:5:A:VAL:HG21	1:9:A:ILE:H	10	0.13
(3,540)	1:5:A:VAL:HG22	1:9:A:ILE:H	10	0.13
(3,540)	1:5:A:VAL:HG23	1:9:A:ILE:H	10	0.13
(3,375)	1:17:A:PRO:HA	1:17:A:PRO:HG2	9	0.13
(3,227)	1:6:A:ARG:H	1:7:A:LEU:H	6	0.13
(3,198)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	7	0.13
(3,198)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	7	0.13
(3,197)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	3	0.13
(3,197)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	3	0.13
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	9	0.13
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	9	0.13
(3,177)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	9	0.13
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	9	0.13
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	9	0.13
(3,177)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	9	0.13
(3,169)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	2	0.13
(3,169)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	4	0.13
(3,129)	1:7:A:LEU:H	1:7:A:LEU:HB3	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,129)	1:7:A:LEU:H	1:7:A:LEU:HB3	7	0.13
(3,122)	1:8:A:TYR:HA	1:12:A:LEU:H	9	0.13
(3,103)	1:7:A:LEU:H	1:10:A:GLN:HB3	3	0.13
(3,98)	1:6:A:ARG:HG3	1:7:A:LEU:H	1	0.13
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD11	2	0.13
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD12	2	0.13
(2,641)	1:5:A:VAL:HG11	1:12:A:LEU:HD13	2	0.13
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD11	2	0.13
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD12	2	0.13
(2,641)	1:5:A:VAL:HG12	1:12:A:LEU:HD13	2	0.13
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD11	2	0.13
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD12	2	0.13
(2,641)	1:5:A:VAL:HG13	1:12:A:LEU:HD13	2	0.13
(2,581)	1:5:A:VAL:HG21	1:9:A:ILE:H	1	0.13
(2,581)	1:5:A:VAL:HG22	1:9:A:ILE:H	1	0.13
(2,581)	1:5:A:VAL:HG23	1:9:A:ILE:H	1	0.13
(2,581)	1:5:A:VAL:HG21	1:9:A:ILE:H	6	0.13
(2,581)	1:5:A:VAL:HG22	1:9:A:ILE:H	6	0.13
(2,581)	1:5:A:VAL:HG23	1:9:A:ILE:H	6	0.13
(2,581)	1:5:A:VAL:HG21	1:9:A:ILE:H	10	0.13
(2,581)	1:5:A:VAL:HG22	1:9:A:ILE:H	10	0.13
(2,581)	1:5:A:VAL:HG23	1:9:A:ILE:H	10	0.13
(2,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	9	0.13
(2,353)	1:9:A:ILE:HB	1:9:A:ILE:HG13	5	0.13
(2,252)	1:6:A:ARG:H	1:7:A:LEU:H	6	0.13
(2,223)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	7	0.13
(2,223)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	7	0.13
(2,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	3	0.13
(2,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	3	0.13
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	9	0.13
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	9	0.13
(2,196)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	9	0.13
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	9	0.13
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	9	0.13
(2,196)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	9	0.13
(2,186)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	2	0.13
(2,186)	1:11:A:TRP:HZ2	1:16:A:GLY:HA3	4	0.13
(2,140)	1:7:A:LEU:H	1:7:A:LEU:HB3	4	0.13
(2,140)	1:7:A:LEU:H	1:7:A:LEU:HB3	7	0.13
(2,133)	1:8:A:TYR:HA	1:12:A:LEU:H	9	0.13
(2,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	3	0.13
(2,106)	1:6:A:ARG:HG3	1:7:A:LEU:H	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG11	2	0.13
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG12	2	0.13
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG13	2	0.13
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG21	1	0.13
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG22	1	0.13
(1,649)	1:2:A:GLU:HB3	1:5:A:VAL:HG23	1	0.13
(1,634)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	1	0.13
(1,634)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	1	0.13
(1,634)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	1	0.13
(1,629)	1:2:A:GLU:HG3	1:5:A:VAL:HB	6	0.13
(1,597)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	7	0.13
(1,583)	1:6:A:ARG:HB3	1:7:A:LEU:H	8	0.13
(1,566)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	3	0.13
(1,566)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	4	0.13
(1,566)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	5	0.13
(1,566)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	6	0.13
(1,566)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	7	0.13
(1,566)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	8	0.13
(1,566)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	9	0.13
(1,566)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	10	0.13
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD11	5	0.13
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD12	5	0.13
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD13	5	0.13
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD21	5	0.13
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD22	5	0.13
(1,553)	1:4:A:CYS:HA	1:7:A:LEU:HD23	5	0.13
(1,540)	1:7:A:LEU:HA	1:10:A:GLN:HB2	8	0.13
(1,529)	1:11:A:TRP:HB3	1:24:A:PRO:HD2	2	0.13
(1,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	0.13
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE2	9	0.13
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE3	9	0.13
(1,514)	1:25:A:CYS:HA	1:25:A:CYS:HB2	7	0.13
(1,505)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	1	0.13
(1,505)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	8	0.13
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	4	0.13
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	4	0.13
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	9	0.13
(1,441)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	9	0.13
(1,436)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	7	0.13
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	5	0.13
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	5	0.13
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	5	0.13
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	5	0.13
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	5	0.13
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	5	0.13
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	5	0.13
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	5	0.13
(1,382)	1:12:A:LEU:HD11	1:12:A:LEU:HG	2	0.13
(1,382)	1:12:A:LEU:HD12	1:12:A:LEU:HG	2	0.13
(1,382)	1:12:A:LEU:HD13	1:12:A:LEU:HG	2	0.13
(1,382)	1:12:A:LEU:HD11	1:12:A:LEU:HG	7	0.13
(1,382)	1:12:A:LEU:HD12	1:12:A:LEU:HG	7	0.13
(1,382)	1:12:A:LEU:HD13	1:12:A:LEU:HG	7	0.13
(1,366)	1:10:A:GLN:HB3	1:10:A:GLN:HG3	2	0.13
(1,306)	1:4:A:CYS:HA	1:4:A:CYS:HB2	9	0.13
(1,255)	1:2:A:GLU:HA	1:3:A:GLU:H	2	0.13
(1,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	1	0.13
(1,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.13
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD11	9	0.13
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD12	9	0.13
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD13	9	0.13
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD21	9	0.13
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD22	9	0.13
(1,141)	1:7:A:LEU:H	1:7:A:LEU:HD23	9	0.13
(1,127)	1:20:A:GLY:HA3	1:21:A:ARG:H	10	0.13
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.13
(1,99)	1:14:A:ASP:H	1:15:A:GLY:H	8	0.13
(1,87)	1:19:A:SER:H	1:19:A:SER:HG	10	0.13
(1,81)	1:4:A:CYS:HA	1:7:A:LEU:H	10	0.13
(1,28)	1:4:A:CYS:H	1:4:A:CYS:HB2	2	0.13
(1,26)	1:3:A:GLU:H	1:3:A:GLU:HG2	8	0.13
(1,26)	1:3:A:GLU:H	1:3:A:GLU:HG3	8	0.13
(4,22)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	4	0.12
(4,22)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	6	0.12
(4,22)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	7	0.12
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	4	0.12
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	4	0.12
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	4	0.12
(4,5)	1:10:A:GLN:H	1:10:A:GLN:HG2	1	0.12
(3,578)	1:5:A:VAL:HA	1:25:A:CYS:HB2	10	0.12
(3,540)	1:5:A:VAL:HG21	1:9:A:ILE:H	9	0.12
(3,540)	1:5:A:VAL:HG22	1:9:A:ILE:H	9	0.12
(3,540)	1:5:A:VAL:HG23	1:9:A:ILE:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,375)	1:17:A:PRO:HA	1:17:A:PRO:HG2	10	0.12
(3,356)	1:12:A:LEU:HG	1:13:A:LYS:H	10	0.12
(3,316)	1:9:A:ILE:HA	1:9:A:ILE:HG13	1	0.12
(3,316)	1:9:A:ILE:HA	1:9:A:ILE:HG13	3	0.12
(3,129)	1:7:A:LEU:H	1:7:A:LEU:HB3	8	0.12
(3,122)	1:8:A:TYR:HA	1:12:A:LEU:H	10	0.12
(3,108)	1:24:A:PRO:HG3	1:25:A:CYS:H	4	0.12
(3,99)	1:9:A:ILE:H	1:9:A:ILE:HG12	7	0.12
(3,95)	1:10:A:GLN:HB2	1:11:A:TRP:H	6	0.12
(3,26)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.12
(3,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	3	0.12
(3,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	5	0.12
(3,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	7	0.12
(2,623)	1:5:A:VAL:HA	1:25:A:CYS:HB2	10	0.12
(2,581)	1:5:A:VAL:HG21	1:9:A:ILE:H	9	0.12
(2,581)	1:5:A:VAL:HG22	1:9:A:ILE:H	9	0.12
(2,581)	1:5:A:VAL:HG23	1:9:A:ILE:H	9	0.12
(2,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	10	0.12
(2,389)	1:12:A:LEU:HG	1:13:A:LYS:H	10	0.12
(2,347)	1:9:A:ILE:HA	1:9:A:ILE:HG13	1	0.12
(2,347)	1:9:A:ILE:HA	1:9:A:ILE:HG13	3	0.12
(2,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	4	0.12
(2,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	6	0.12
(2,209)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	7	0.12
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	4	0.12
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	4	0.12
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	4	0.12
(2,140)	1:7:A:LEU:H	1:7:A:LEU:HB3	8	0.12
(2,133)	1:8:A:TYR:HA	1:12:A:LEU:H	10	0.12
(2,117)	1:24:A:PRO:HG3	1:25:A:CYS:H	4	0.12
(2,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	7	0.12
(2,103)	1:10:A:GLN:HB2	1:11:A:TRP:H	6	0.12
(2,31)	1:10:A:GLN:H	1:10:A:GLN:HG2	1	0.12
(2,30)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.12
(2,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	3	0.12
(2,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	5	0.12
(2,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	7	0.12
(1,629)	1:2:A:GLU:HG3	1:5:A:VAL:HB	5	0.12
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB2	9	0.12
(1,621)	1:10:A:GLN:HA	1:13:A:LYS:HB3	9	0.12
(1,589)	1:23:A:PRO:HA	1:25:A:CYS:H	7	0.12
(1,576)	1:10:A:GLN:H	1:12:A:LEU:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:23:A:PRO:HA	1:24:A:PRO:HD2	9	0.12
(1,566)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	1	0.12
(1,566)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	2	0.12
(1,550)	1:8:A:TYR:HA	1:11:A:TRP:HB3	7	0.12
(1,527)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.12
(1,505)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	3	0.12
(1,505)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	4	0.12
(1,505)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	5	0.12
(1,505)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	6	0.12
(1,505)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	7	0.12
(1,456)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	3	0.12
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	1	0.12
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	1	0.12
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	2	0.12
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	2	0.12
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	6	0.12
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	6	0.12
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	8	0.12
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	8	0.12
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	9	0.12
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	9	0.12
(1,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	5	0.12
(1,408)	1:17:A:PRO:HA	1:17:A:PRO:HG3	5	0.12
(1,395)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	10	0.12
(1,395)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	10	0.12
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	7	0.12
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	7	0.12
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	7	0.12
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	7	0.12
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	7	0.12
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	7	0.12
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	7	0.12
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	7	0.12
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	7	0.12
(1,375)	1:12:A:LEU:HA	1:12:A:LEU:HB3	7	0.12
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	5	0.12
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	5	0.12
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	5	0.12
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	7	0.12
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	7	0.12
(1,357)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	7	0.12
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG11	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG12	9	0.12
(1,311)	1:5:A:VAL:HA	1:5:A:VAL:HG13	9	0.12
(1,288)	1:12:A:LEU:HA	1:16:A:GLY:H	9	0.12
(1,258)	1:14:A:ASP:HB3	1:16:A:GLY:H	1	0.12
(1,255)	1:2:A:GLU:HA	1:3:A:GLU:H	7	0.12
(1,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	1	0.12
(1,205)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	1	0.12
(1,205)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	1	0.12
(1,202)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	6	0.12
(1,202)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	6	0.12
(1,202)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	10	0.12
(1,202)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	10	0.12
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	2	0.12
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	2	0.12
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	2	0.12
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	2	0.12
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	2	0.12
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	2	0.12
(1,158)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	9	0.12
(1,150)	1:8:A:TYR:HD1	1:9:A:ILE:HA	5	0.12
(1,150)	1:8:A:TYR:HD2	1:9:A:ILE:HA	5	0.12
(1,104)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.12
(1,104)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.12
(1,104)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.12
(1,99)	1:14:A:ASP:H	1:15:A:GLY:H	9	0.12
(1,87)	1:19:A:SER:H	1:19:A:SER:HG	5	0.12
(1,45)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	2	0.12
(1,45)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	10	0.12
(1,41)	1:14:A:ASP:H	1:14:A:ASP:HB2	1	0.12
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD11	2	0.11
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD12	2	0.11
(4,41)	1:9:A:ILE:HA	1:12:A:LEU:HD13	2	0.11
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	9	0.11
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	9	0.11
(4,18)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	9	0.11
(4,5)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.11
(4,3)	1:12:A:LEU:HD21	1:13:A:LYS:H	9	0.11
(4,3)	1:12:A:LEU:HD22	1:13:A:LYS:H	9	0.11
(4,3)	1:12:A:LEU:HD23	1:13:A:LYS:H	9	0.11
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG11	7	0.11
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG12	7	0.11
(4,2)	1:5:A:VAL:H	1:5:A:VAL:HG13	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,578)	1:5:A:VAL:HA	1:25:A:CYS:HB2	1	0.11
(3,578)	1:5:A:VAL:HA	1:25:A:CYS:HB2	3	0.11
(3,540)	1:5:A:VAL:HG21	1:9:A:ILE:H	2	0.11
(3,540)	1:5:A:VAL:HG22	1:9:A:ILE:H	2	0.11
(3,540)	1:5:A:VAL:HG23	1:9:A:ILE:H	2	0.11
(3,540)	1:5:A:VAL:HG21	1:9:A:ILE:H	8	0.11
(3,540)	1:5:A:VAL:HG22	1:9:A:ILE:H	8	0.11
(3,540)	1:5:A:VAL:HG23	1:9:A:ILE:H	8	0.11
(3,518)	1:9:A:ILE:HG21	1:10:A:GLN:HA	8	0.11
(3,518)	1:9:A:ILE:HG22	1:10:A:GLN:HA	8	0.11
(3,518)	1:9:A:ILE:HG23	1:10:A:GLN:HA	8	0.11
(3,431)	1:23:A:PRO:HA	1:23:A:PRO:HG2	3	0.11
(3,431)	1:23:A:PRO:HA	1:23:A:PRO:HG2	6	0.11
(3,431)	1:23:A:PRO:HA	1:23:A:PRO:HG2	7	0.11
(3,431)	1:23:A:PRO:HA	1:23:A:PRO:HG2	9	0.11
(3,375)	1:17:A:PRO:HA	1:17:A:PRO:HG2	4	0.11
(3,375)	1:17:A:PRO:HA	1:17:A:PRO:HG2	7	0.11
(3,356)	1:12:A:LEU:HG	1:13:A:LYS:H	3	0.11
(3,356)	1:12:A:LEU:HG	1:13:A:LYS:H	6	0.11
(3,214)	1:15:A:GLY:HA2	1:16:A:GLY:H	8	0.11
(3,197)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	6	0.11
(3,197)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	6	0.11
(3,197)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	9	0.11
(3,197)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	9	0.11
(3,195)	1:8:A:TYR:HE1	1:12:A:LEU:HG	6	0.11
(3,195)	1:8:A:TYR:HE2	1:12:A:LEU:HG	6	0.11
(3,189)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	8	0.11
(3,129)	1:7:A:LEU:H	1:7:A:LEU:HB3	3	0.11
(3,27)	1:10:A:GLN:H	1:10:A:GLN:HB3	7	0.11
(3,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	2	0.11
(2,623)	1:5:A:VAL:HA	1:25:A:CYS:HB2	1	0.11
(2,623)	1:5:A:VAL:HA	1:25:A:CYS:HB2	3	0.11
(2,581)	1:5:A:VAL:HG21	1:9:A:ILE:H	2	0.11
(2,581)	1:5:A:VAL:HG22	1:9:A:ILE:H	2	0.11
(2,581)	1:5:A:VAL:HG23	1:9:A:ILE:H	2	0.11
(2,581)	1:5:A:VAL:HG21	1:9:A:ILE:H	8	0.11
(2,581)	1:5:A:VAL:HG22	1:9:A:ILE:H	8	0.11
(2,581)	1:5:A:VAL:HG23	1:9:A:ILE:H	8	0.11
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD11	2	0.11
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD12	2	0.11
(2,575)	1:9:A:ILE:HA	1:12:A:LEU:HD13	2	0.11
(2,556)	1:9:A:ILE:HG21	1:10:A:GLN:HA	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,556)	1:9:A:ILE:HG22	1:10:A:GLN:HA	8	0.11
(2,556)	1:9:A:ILE:HG23	1:10:A:GLN:HA	8	0.11
(2,465)	1:23:A:PRO:HA	1:23:A:PRO:HG2	3	0.11
(2,465)	1:23:A:PRO:HA	1:23:A:PRO:HG2	6	0.11
(2,465)	1:23:A:PRO:HA	1:23:A:PRO:HG2	7	0.11
(2,465)	1:23:A:PRO:HA	1:23:A:PRO:HG2	9	0.11
(2,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	4	0.11
(2,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	7	0.11
(2,389)	1:12:A:LEU:HG	1:13:A:LYS:H	3	0.11
(2,389)	1:12:A:LEU:HG	1:13:A:LYS:H	6	0.11
(2,239)	1:15:A:GLY:HA2	1:16:A:GLY:H	8	0.11
(2,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	6	0.11
(2,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	6	0.11
(2,221)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	9	0.11
(2,221)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	9	0.11
(2,219)	1:8:A:TYR:HE1	1:12:A:LEU:HG	6	0.11
(2,219)	1:8:A:TYR:HE2	1:12:A:LEU:HG	6	0.11
(2,211)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	8	0.11
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	9	0.11
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	9	0.11
(2,190)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	9	0.11
(2,140)	1:7:A:LEU:H	1:7:A:LEU:HB3	3	0.11
(2,32)	1:10:A:GLN:H	1:10:A:GLN:HB3	7	0.11
(2,31)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.11
(2,12)	1:12:A:LEU:HD21	1:13:A:LYS:H	9	0.11
(2,12)	1:12:A:LEU:HD22	1:13:A:LYS:H	9	0.11
(2,12)	1:12:A:LEU:HD23	1:13:A:LYS:H	9	0.11
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG11	7	0.11
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG12	7	0.11
(2,7)	1:5:A:VAL:H	1:5:A:VAL:HG13	7	0.11
(2,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	2	0.11
(1,670)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	4	0.11
(1,670)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	4	0.11
(1,590)	1:24:A:PRO:HB2	1:25:A:CYS:H	1	0.11
(1,576)	1:10:A:GLN:H	1:12:A:LEU:H	5	0.11
(1,576)	1:10:A:GLN:H	1:12:A:LEU:H	6	0.11
(1,569)	1:23:A:PRO:HA	1:24:A:PRO:HD3	9	0.11
(1,456)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	1	0.11
(1,456)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	2	0.11
(1,436)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	6	0.11
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	3	0.11
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	4	0.11
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	4	0.11
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	5	0.11
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	5	0.11
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	7	0.11
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	7	0.11
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	10	0.11
(1,417)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	10	0.11
(1,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	3	0.11
(1,408)	1:17:A:PRO:HA	1:17:A:PRO:HG3	3	0.11
(1,395)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	6	0.11
(1,395)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	6	0.11
(1,388)	1:12:A:LEU:HB2	1:13:A:LYS:H	4	0.11
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	2	0.11
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	2	0.11
(1,387)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	2	0.11
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	2	0.11
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	2	0.11
(1,387)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	2	0.11
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	2	0.11
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	2	0.11
(1,387)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	2	0.11
(1,366)	1:10:A:GLN:HB3	1:10:A:GLN:HG3	5	0.11
(1,336)	1:7:A:LEU:HA	1:7:A:LEU:HB3	5	0.11
(1,336)	1:7:A:LEU:HA	1:7:A:LEU:HB3	7	0.11
(1,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	0.11
(1,213)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	0.11
(1,202)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	9	0.11
(1,202)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	9	0.11
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	1	0.11
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	1	0.11
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	1	0.11
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	1	0.11
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	1	0.11
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	1	0.11
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	7	0.11
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	7	0.11
(1,200)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	7	0.11
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	7	0.11
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	7	0.11
(1,200)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	7	0.11
(4,32)	1:9:A:ILE:HB	1:9:A:ILE:HG13	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,611)	1:6:A:ARG:HA	1:9:A:ILE:HG12	9	0.1
(3,540)	1:5:A:VAL:HG21	1:9:A:ILE:H	7	0.1
(3,540)	1:5:A:VAL:HG22	1:9:A:ILE:H	7	0.1
(3,540)	1:5:A:VAL:HG23	1:9:A:ILE:H	7	0.1
(3,518)	1:9:A:ILE:HG21	1:10:A:GLN:HA	3	0.1
(3,518)	1:9:A:ILE:HG22	1:10:A:GLN:HA	3	0.1
(3,518)	1:9:A:ILE:HG23	1:10:A:GLN:HA	3	0.1
(3,481)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	5	0.1
(3,481)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	5	0.1
(3,481)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	5	0.1
(3,431)	1:23:A:PRO:HA	1:23:A:PRO:HG2	10	0.1
(3,375)	1:17:A:PRO:HA	1:17:A:PRO:HG2	3	0.1
(3,316)	1:9:A:ILE:HA	1:9:A:ILE:HG13	6	0.1
(3,316)	1:9:A:ILE:HA	1:9:A:ILE:HG13	8	0.1
(3,316)	1:9:A:ILE:HA	1:9:A:ILE:HG13	10	0.1
(3,246)	1:12:A:LEU:H	1:12:A:LEU:HD21	8	0.1
(3,246)	1:12:A:LEU:H	1:12:A:LEU:HD22	8	0.1
(3,246)	1:12:A:LEU:H	1:12:A:LEU:HD23	8	0.1
(3,246)	1:12:A:LEU:H	1:12:A:LEU:HD21	9	0.1
(3,246)	1:12:A:LEU:H	1:12:A:LEU:HD22	9	0.1
(3,246)	1:12:A:LEU:H	1:12:A:LEU:HD23	9	0.1
(3,241)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	1	0.1
(3,241)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	2	0.1
(3,241)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	8	0.1
(3,195)	1:8:A:TYR:HE1	1:12:A:LEU:HG	5	0.1
(3,195)	1:8:A:TYR:HE2	1:12:A:LEU:HG	5	0.1
(3,195)	1:8:A:TYR:HE1	1:12:A:LEU:HG	10	0.1
(3,195)	1:8:A:TYR:HE2	1:12:A:LEU:HG	10	0.1
(3,189)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	5	0.1
(3,141)	1:11:A:TRP:HD1	1:19:A:SER:HB3	10	0.1
(3,129)	1:7:A:LEU:H	1:7:A:LEU:HB3	5	0.1
(3,108)	1:24:A:PRO:HG3	1:25:A:CYS:H	7	0.1
(3,103)	1:7:A:LEU:H	1:10:A:GLN:HB3	6	0.1
(3,27)	1:10:A:GLN:H	1:10:A:GLN:HB3	5	0.1
(3,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	1	0.1
(3,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	8	0.1
(2,662)	1:6:A:ARG:HA	1:9:A:ILE:HG12	9	0.1
(2,581)	1:5:A:VAL:HG21	1:9:A:ILE:H	7	0.1
(2,581)	1:5:A:VAL:HG22	1:9:A:ILE:H	7	0.1
(2,581)	1:5:A:VAL:HG23	1:9:A:ILE:H	7	0.1
(2,556)	1:9:A:ILE:HG21	1:10:A:GLN:HA	3	0.1
(2,556)	1:9:A:ILE:HG22	1:10:A:GLN:HA	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,556)	1:9:A:ILE:HG23	1:10:A:GLN:HA	3	0.1
(2,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	5	0.1
(2,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	5	0.1
(2,518)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	5	0.1
(2,465)	1:23:A:PRO:HA	1:23:A:PRO:HG2	10	0.1
(2,408)	1:17:A:PRO:HA	1:17:A:PRO:HG2	3	0.1
(2,353)	1:9:A:ILE:HB	1:9:A:ILE:HG13	2	0.1
(2,347)	1:9:A:ILE:HA	1:9:A:ILE:HG13	6	0.1
(2,347)	1:9:A:ILE:HA	1:9:A:ILE:HG13	8	0.1
(2,347)	1:9:A:ILE:HA	1:9:A:ILE:HG13	10	0.1
(2,272)	1:12:A:LEU:H	1:12:A:LEU:HD21	8	0.1
(2,272)	1:12:A:LEU:H	1:12:A:LEU:HD22	8	0.1
(2,272)	1:12:A:LEU:H	1:12:A:LEU:HD23	8	0.1
(2,272)	1:12:A:LEU:H	1:12:A:LEU:HD21	9	0.1
(2,272)	1:12:A:LEU:H	1:12:A:LEU:HD22	9	0.1
(2,272)	1:12:A:LEU:H	1:12:A:LEU:HD23	9	0.1
(2,266)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	1	0.1
(2,266)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	2	0.1
(2,266)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	8	0.1
(2,219)	1:8:A:TYR:HE1	1:12:A:LEU:HG	5	0.1
(2,219)	1:8:A:TYR:HE2	1:12:A:LEU:HG	5	0.1
(2,219)	1:8:A:TYR:HE1	1:12:A:LEU:HG	10	0.1
(2,219)	1:8:A:TYR:HE2	1:12:A:LEU:HG	10	0.1
(2,211)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	5	0.1
(2,152)	1:11:A:TRP:HD1	1:19:A:SER:HB3	10	0.1
(2,140)	1:7:A:LEU:H	1:7:A:LEU:HB3	5	0.1
(2,117)	1:24:A:PRO:HG3	1:25:A:CYS:H	7	0.1
(2,112)	1:7:A:LEU:H	1:10:A:GLN:HB3	6	0.1
(2,32)	1:10:A:GLN:H	1:10:A:GLN:HB3	5	0.1
(2,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	1	0.1
(2,3)	1:16:A:GLY:H	1:16:A:GLY:HA3	8	0.1
(1,670)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	2	0.1
(1,670)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	2	0.1
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	4	0.1
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	4	0.1
(1,644)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	4	0.1
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	4	0.1
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	4	0.1
(1,644)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	4	0.1
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	4	0.1
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	4	0.1
(1,644)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,591)	1:2:A:GLU:HB2	1:5:A:VAL:H	10	0.1
(1,576)	1:10:A:GLN:H	1:12:A:LEU:H	10	0.1
(1,570)	1:23:A:PRO:HA	1:24:A:PRO:HD2	1	0.1
(1,542)	1:11:A:TRP:HA	1:14:A:ASP:HB3	6	0.1
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE2	2	0.1
(1,519)	1:13:A:LYS:HA	1:13:A:LYS:HE3	2	0.1
(1,436)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	10	0.1
(1,304)	1:3:A:GLU:HA	1:3:A:GLU:HB2	8	0.1
(1,304)	1:3:A:GLU:HA	1:3:A:GLU:HB3	8	0.1
(1,222)	1:8:A:TYR:HE1	1:9:A:ILE:HG12	1	0.1
(1,222)	1:8:A:TYR:HE2	1:9:A:ILE:HG12	1	0.1
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	2	0.1
(1,114)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	2	0.1
(1,109)	1:12:A:LEU:H	1:12:A:LEU:HB2	5	0.1
(1,86)	1:18:A:SER:HA	1:19:A:SER:H	7	0.1
(1,80)	1:5:A:VAL:HA	1:8:A:TYR:H	5	0.1
(1,43)	1:4:A:CYS:HB3	1:5:A:VAL:H	10	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found