



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 01:33 PM UTC

PDB ID : 9GDN / pdb_00009gdn
BMRB ID : 34943
Title : Trp-cage fortified Tc5b-Exenatide chimera with disulfide bond cyclization (Ex-4-Tc5bCC) at 288K
Authors : Horvath, D.
Deposited on : 2024-08-06

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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

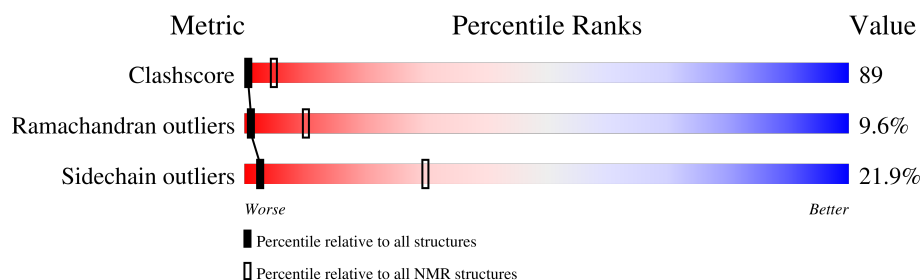
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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	

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:2-A:25 (24)	0.30	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 1 clusters and 2 single-model clusters were found.

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

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-Tc5bSS).

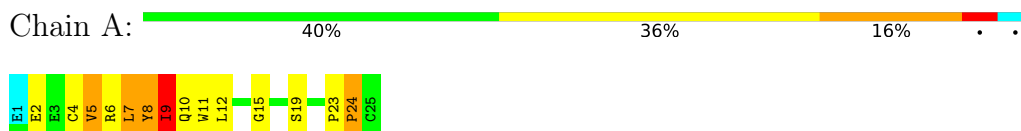
Mol	Chain	Residues	Atoms						Trace
1	A	25	Total	C	H	N	O	S	0
			384	123	187	34	38	2	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)

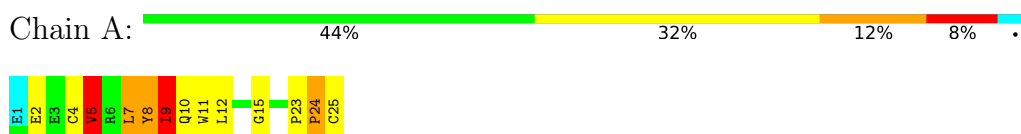


4.2 Scores per residue for each member of the ensemble

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

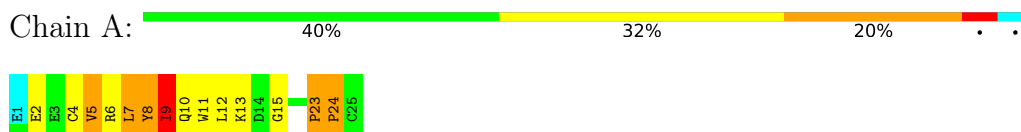
4.2.1 Score per residue for model 1

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



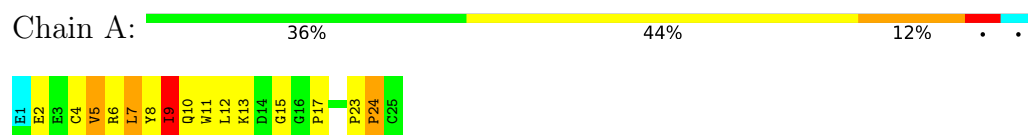
4.2.2 Score per residue for model 2

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



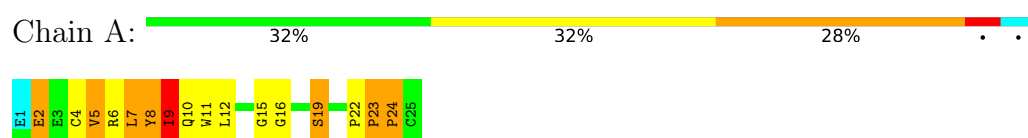
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



4.2.4 Score per residue for model 4

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



4.2.5 Score per residue for model 5

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



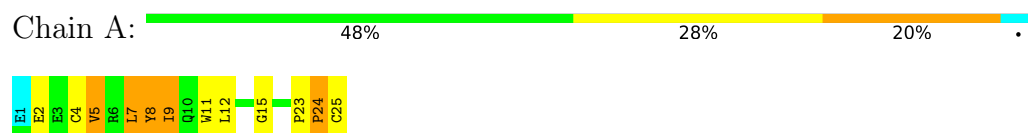
4.2.6 Score per residue for model 6

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



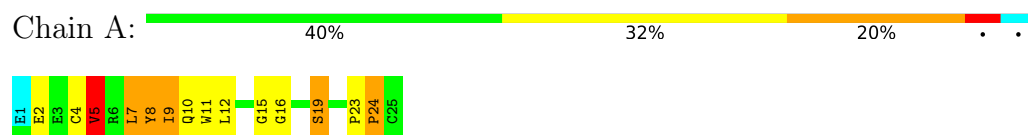
4.2.7 Score per residue for model 7

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



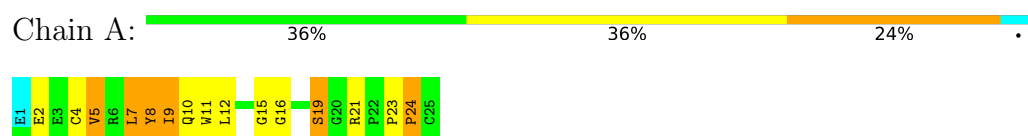
4.2.8 Score per residue for model 8

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



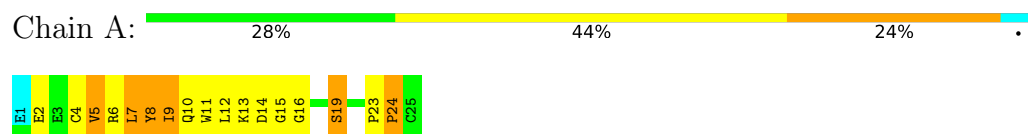
4.2.9 Score per residue for model 9

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



4.2.10 Score per residue for model 10

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bSS)



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	167
Number of shifts mapped to atoms	167
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.36±0.07	2±1/194 (1.2± 0.6%)	1.29±0.08	0±1/262 (0.2± 0.3%)
All	All	1.36	23/1940 (1.2%)	1.29	4/2620 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	8	TYR	CE1-CZ	7.36	1.55	1.38	8	4
1	A	8	TYR	CE2-CZ	-6.47	1.22	1.38	8	3
1	A	8	TYR	CA-C	-6.19	1.46	1.53	1	5
1	A	8	TYR	C-N	-5.57	1.27	1.34	10	4
1	A	9	ILE	N-CA	-5.35	1.40	1.46	2	5
1	A	5	VAL	C-N	-5.09	1.27	1.33	1	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	PRO	O-C-N	6.75	124.41	121.31	4	2
1	A	22	PRO	CA-C-N	5.90	123.97	119.66	4	1
1	A	22	PRO	C-N-CA	5.90	123.97	119.66	4	1

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	188	179	179	33±2
All	All	1880	1790	1790	328

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 89.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:HD11	1:A:25:CYS:SG	0.94	2.02	6	1
1:A:7:LEU:HD12	1:A:24:PRO:HB2	0.81	1.53	8	9
1:A:4:CYS:O	1:A:7:LEU:HG	0.77	1.79	7	10
1:A:5:VAL:O	1:A:9:ILE:HG13	0.72	1.84	1	10
1:A:16:GLY:O	1:A:19:SER:HB3	0.72	1.84	9	4
1:A:5:VAL:O	1:A:8:TYR:HB3	0.71	1.86	3	10
1:A:8:TYR:O	1:A:11:TRP:HB3	0.69	1.86	10	10
1:A:8:TYR:HA	1:A:24:PRO:CG	0.69	2.18	10	10
1:A:11:TRP:CE3	1:A:12:LEU:HD12	0.66	2.26	1	10
1:A:8:TYR:HA	1:A:24:PRO:HG2	0.66	1.67	10	10
1:A:4:CYS:HA	1:A:7:LEU:HD21	0.66	1.66	7	9
1:A:7:LEU:CD1	1:A:24:PRO:HB2	0.65	2.22	2	8
1:A:4:CYS:HA	1:A:7:LEU:CD2	0.64	2.22	2	8
1:A:2:GLU:HB2	1:A:5:VAL:HB	0.63	1.70	8	10
1:A:11:TRP:HE3	1:A:12:LEU:HD12	0.63	1.54	2	10
1:A:5:VAL:HA	1:A:8:TYR:HB3	0.62	1.70	1	3
1:A:8:TYR:CE2	1:A:12:LEU:HD11	0.62	2.30	2	10
1:A:8:TYR:CE2	1:A:12:LEU:HD21	0.62	2.30	10	10
1:A:8:TYR:CZ	1:A:12:LEU:HD11	0.60	2.32	2	10
1:A:11:TRP:CZ3	1:A:23:PRO:HB3	0.58	2.33	6	9
1:A:5:VAL:HG13	1:A:9:ILE:HG13	0.58	1.75	2	8
1:A:11:TRP:HE3	1:A:12:LEU:CD1	0.57	2.12	8	10
1:A:11:TRP:CZ2	1:A:23:PRO:HD3	0.57	2.35	4	10
1:A:9:ILE:HA	1:A:12:LEU:HB2	0.56	1.78	10	10
1:A:5:VAL:HG13	1:A:9:ILE:CG1	0.56	2.31	1	6
1:A:11:TRP:CE3	1:A:12:LEU:CD1	0.55	2.90	8	10
1:A:5:VAL:HA	1:A:8:TYR:CB	0.54	2.32	1	3
1:A:8:TYR:O	1:A:12:LEU:HD13	0.51	2.05	1	10
1:A:8:TYR:C	1:A:12:LEU:HD13	0.51	2.30	1	10
1:A:7:LEU:HD13	1:A:24:PRO:HB2	0.51	1.82	6	1
1:A:9:ILE:O	1:A:12:LEU:HB2	0.49	2.07	2	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:CYS:C	1:A:7:LEU:HG	0.49	2.33	8	6
1:A:7:LEU:O	1:A:24:PRO:HG3	0.49	2.08	10	8
1:A:4:CYS:HA	1:A:7:LEU:CG	0.48	2.37	2	6
1:A:9:ILE:O	1:A:13:LYS:N	0.47	2.46	6	5
1:A:5:VAL:C	1:A:8:TYR:HB3	0.47	2.34	1	1
1:A:8:TYR:O	1:A:11:TRP:N	0.46	2.48	1	9
1:A:5:VAL:CA	1:A:8:TYR:HB3	0.46	2.37	1	1
1:A:5:VAL:HG13	1:A:9:ILE:CD1	0.46	2.41	6	3
1:A:2:GLU:H	1:A:2:GLU:CD	0.45	2.18	4	1
1:A:4:CYS:HB2	1:A:25:CYS:HA	0.45	1.89	1	1
1:A:15:GLY:C	1:A:19:SER:HB3	0.44	2.36	6	1
1:A:9:ILE:HA	1:A:12:LEU:HD13	0.44	1.89	2	8
1:A:11:TRP:O	1:A:14:ASP:HB2	0.44	2.13	5	1
1:A:5:VAL:HG12	1:A:6:ARG:N	0.44	2.28	6	2
1:A:14:ASP:HB3	1:A:19:SER:HB2	0.44	1.90	10	1
1:A:4:CYS:HA	1:A:7:LEU:HG	0.43	1.91	2	4
1:A:4:CYS:O	1:A:8:TYR:HB2	0.42	2.14	1	2
1:A:2:GLU:CB	1:A:5:VAL:HB	0.42	2.44	2	1
1:A:12:LEU:HD12	1:A:12:LEU:N	0.42	2.29	5	1
1:A:2:GLU:O	1:A:6:ARG:HB2	0.41	2.14	3	4
1:A:5:VAL:CG1	1:A:9:ILE:HG13	0.41	2.43	2	1
1:A:4:CYS:O	1:A:25:CYS:HB2	0.41	2.16	7	1
1:A:9:ILE:HA	1:A:12:LEU:HD22	0.41	1.93	1	1
1:A:4:CYS:SG	1:A:5:VAL:N	0.41	2.94	8	1
1:A:8:TYR:CE2	1:A:12:LEU:CD2	0.41	3.04	10	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	23/25 (92%)	18±1 (79±6%)	3±1 (11±5%)	2±0 (10±2%)	1	10
All	All	230/250 (92%)	182 (79%)	26 (11%)	22 (10%)	1	10

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	15	GLY	10
1	A	24	PRO	10
1	A	17	PRO	1
1	A	2	GLU	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	21/22 (95%)	16±1 (78±4%)	5±1 (22±4%)	2	30
All	All	210/220 (95%)	164 (78%)	46 (22%)	2	30

All 8 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	5	VAL	10
1	A	9	ILE	10
1	A	7	LEU	9
1	A	10	GLN	9
1	A	19	SER	4
1	A	21	ARG	2
1	A	2	GLU	1
1	A	4	CYS	1

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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 51% 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_288K_20160427*

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	167
Number of shifts mapped to atoms	167
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 51%, i.e. 161 atoms were assigned a chemical shift out of a possible 316. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	46/115 (40%)	46/47 (98%)	0/48 (0%)	0/20 (0%)
Sidechain	105/180 (58%)	105/116 (91%)	0/56 (0%)	0/8 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	161/316 (51%)	161/173 (93%)	0/114 (0%)	0/29 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 166 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	109/187 (58%)	109/120 (91%)	0/59 (0%)	0/8 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	166/328 (51%)	166/179 (93%)	0/119 (0%)	0/30 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

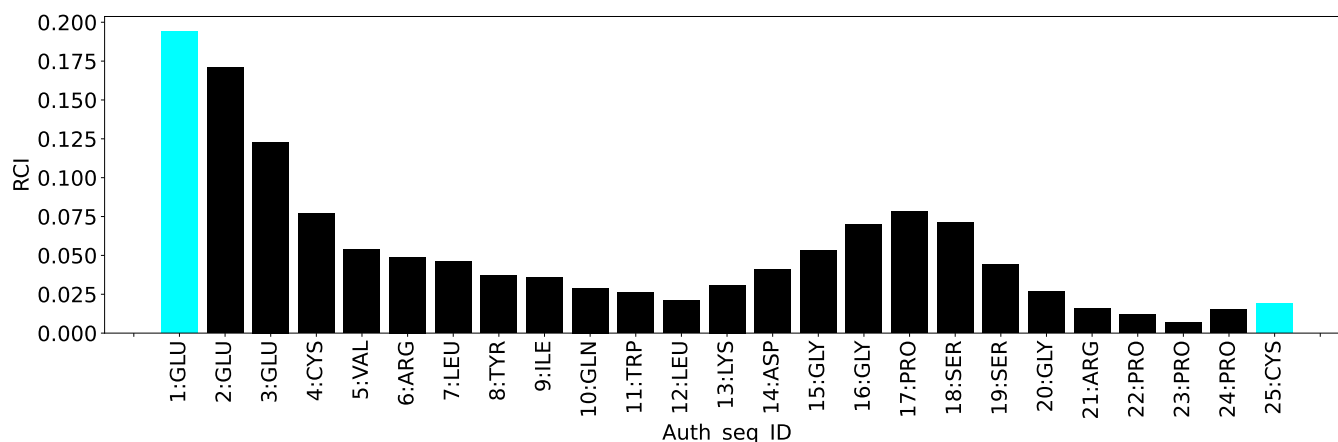
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	16	GLY	HA2	0.58	2.15 – 5.77	-9.3
2	A	23	PRO	HA	2.21	2.78 – 6.00	-6.8

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	2253
Intra-residue ($ i-j =0$)	983
Sequential ($ i-j =1$)	506
Medium range ($ i-j >1$ and $ i-j <5$)	411
Long range ($ i-j \geq 5$)	353
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	90.1
Number of long range restraints per residue ¹	14.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	106.8	0.2
0.2-0.5 (Medium)	179.5	0.5
>0.5 (Large)	181.6	4.46

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 ⓘ

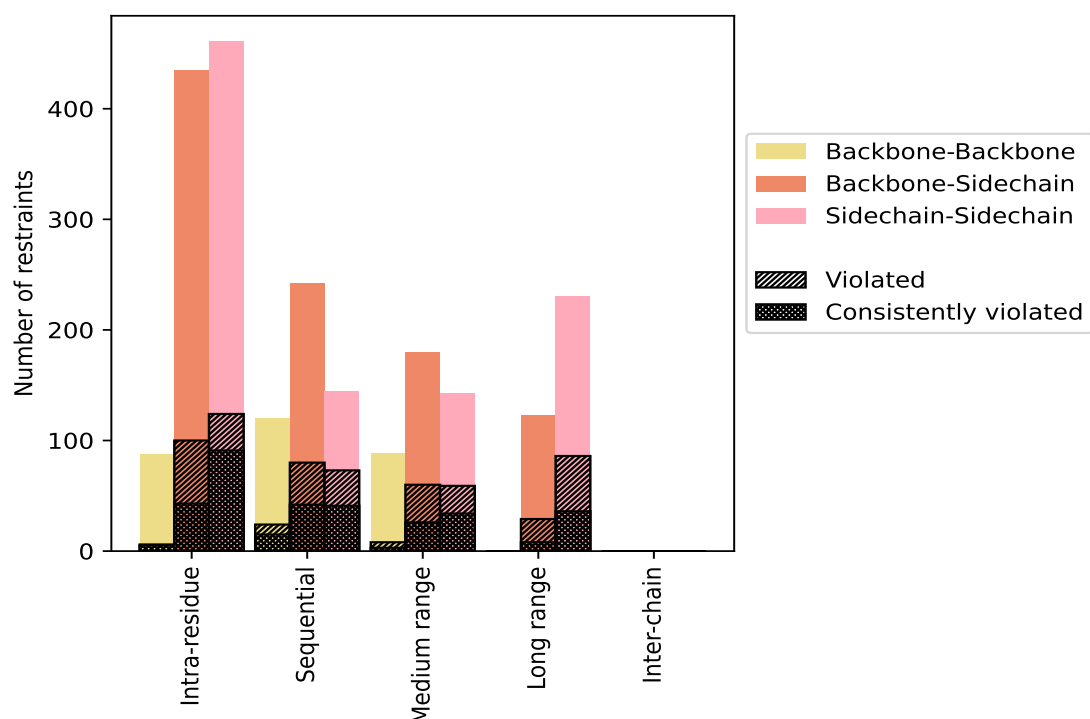
9.1 Summary of distance violations ⓘ

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)	983	43.6	230	23.4	10.2	139	14.1	6.2
Backbone-Backbone	87	3.9	6	6.9	0.3	5	5.7	0.2
Backbone-Sidechain	435	19.3	100	23.0	4.4	43	9.9	1.9
Sidechain-Sidechain	461	20.5	124	26.9	5.5	91	19.7	4.0
Sequential (i-j =1)	506	22.5	177	35.0	7.9	98	19.4	4.3
Backbone-Backbone	120	5.3	24	20.0	1.1	15	12.5	0.7
Backbone-Sidechain	242	10.7	80	33.1	3.6	42	17.4	1.9
Sidechain-Sidechain	144	6.4	73	50.7	3.2	41	28.5	1.8
Medium range (i-j >1 & i-j <5)	411	18.2	127	30.9	5.6	63	15.3	2.8
Backbone-Backbone	88	3.9	8	9.1	0.4	3	3.4	0.1
Backbone-Sidechain	180	8.0	60	33.3	2.7	26	14.4	1.2
Sidechain-Sidechain	143	6.3	59	41.3	2.6	34	23.8	1.5
Long range (i-j ≥5)	353	15.7	115	32.6	5.1	44	12.5	2.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	123	5.5	29	23.6	1.3	8	6.5	0.4
Sidechain-Sidechain	230	10.2	86	37.4	3.8	36	15.7	1.6
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	2253	100.0	649	28.8	28.8	344	15.3	15.3
Backbone-Backbone	295	13.1	38	12.9	1.7	23	7.8	1.0
Backbone-Sidechain	980	43.5	269	27.4	11.9	119	12.1	5.3
Sidechain-Sidechain	978	43.4	342	35.0	15.2	202	20.7	9.0

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

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



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

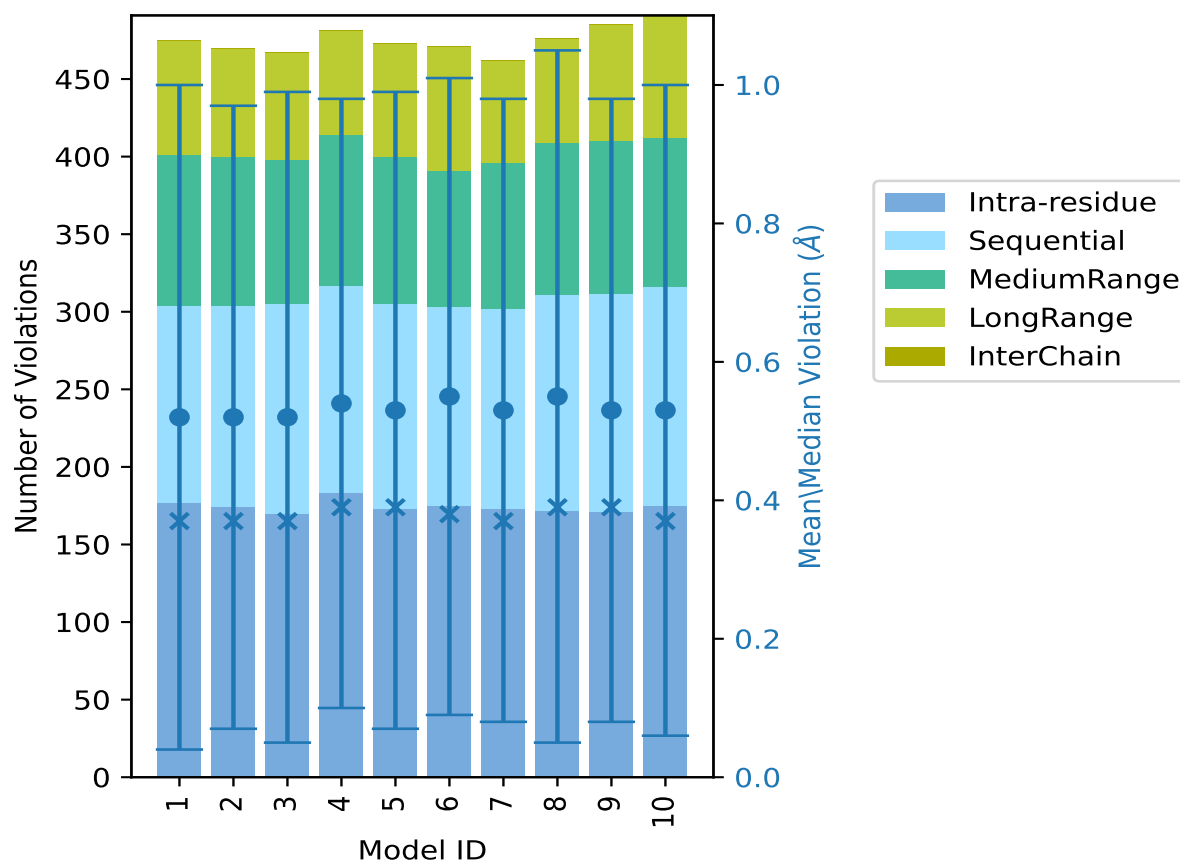
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	177	127	97	74	0	475	0.52	4.46	0.48	0.37
2	174	130	96	70	0	470	0.52	3.22	0.45	0.37
3	170	135	93	69	0	467	0.52	3.9	0.47	0.37
4	183	134	97	67	0	481	0.54	3.2	0.44	0.39
5	173	132	95	73	0	473	0.53	3.14	0.46	0.39
6	175	128	88	80	0	471	0.55	3.18	0.46	0.38
7	173	129	94	66	0	462	0.53	3.03	0.45	0.37
8	172	139	98	67	0	476	0.55	4.28	0.5	0.39
9	171	141	98	75	0	485	0.53	3.05	0.45	0.39
10	175	141	96	79	0	491	0.53	2.92	0.47	0.37

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, 1604(IR:753, SQ:329, MR:284, LR:238, 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	%
24	17	8	21	0	70	1	10.0
14	13	12	13	0	52	2	20.0
10	9	6	4	0	29	3	30.0

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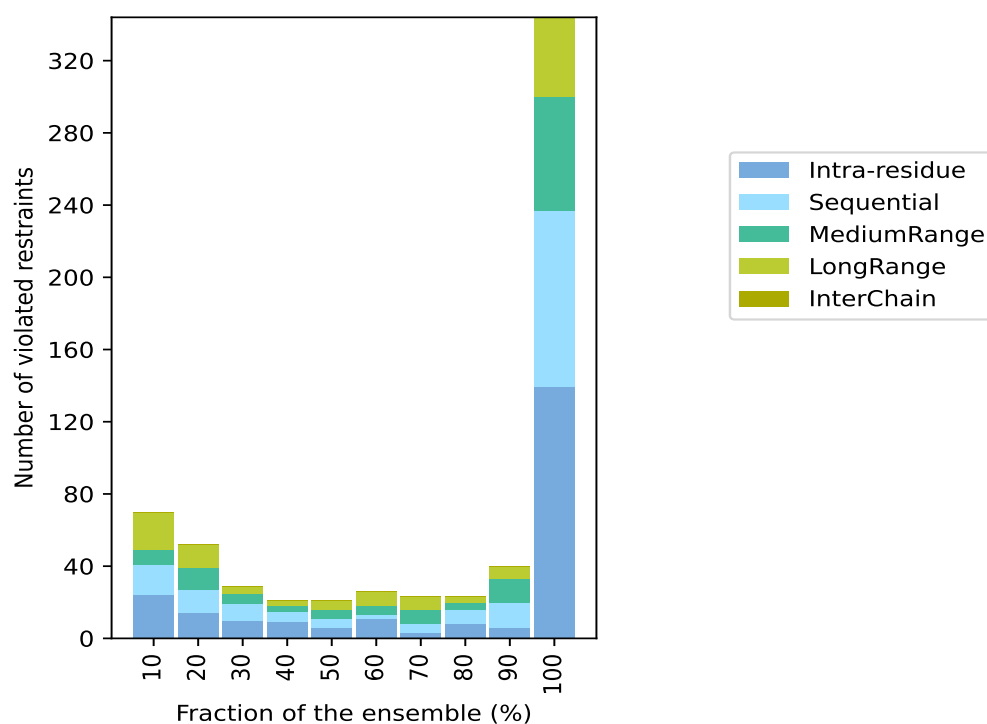
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
9	6	3	3	0	21	4	40.0
6	5	5	5	0	21	5	50.0
11	2	5	8	0	26	6	60.0
3	5	8	7	0	23	7	70.0
8	8	4	3	0	23	8	80.0
6	14	13	7	0	40	9	90.0
139	98	63	44	0	344	10	100.0

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

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

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

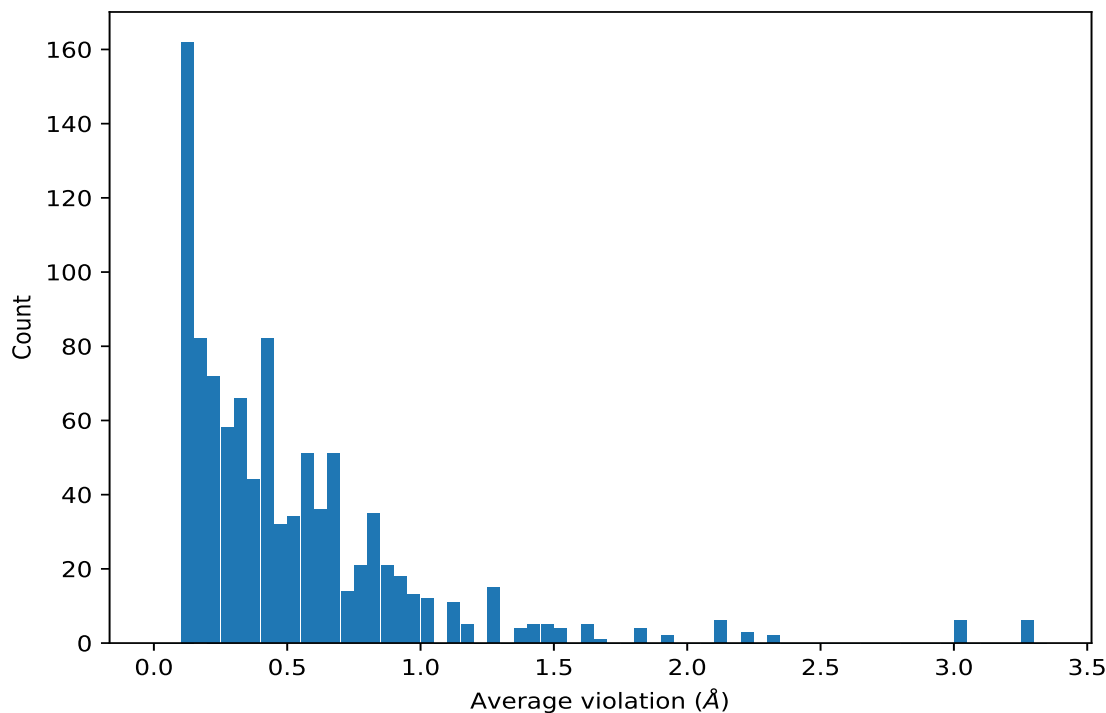


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	10	3.28	0.63	3.14
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	10	3.28	0.63	3.14
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	10	3.28	0.63	3.14
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	10	3.28	0.63	3.14
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	10	3.28	0.63	3.14
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	10	3.28	0.63	3.14
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	10	3.05	0.59	2.86
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	10	3.05	0.59	2.86
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	10	3.05	0.59	2.86
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	10	3.05	0.59	2.86
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	10	3.05	0.59	2.86
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	10	3.05	0.59	2.86
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG2	10	2.31	0.15	2.34
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG3	10	2.31	0.15	2.34
(1,636)	1:10:A:GLN:HA	1:11:A:TRP:HB2	10	2.24	0.03	2.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,60)	1:10:A:GLN:HA	1:11:A:TRP:HB2	10	2.24	0.03	2.26
(2,597)	1:21:A:ARG:HB3	1:21:A:ARG:HE	10	2.22	0.48	2.02
(1,720)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	2.12	0.25	2.24
(1,720)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	2.12	0.25	2.24
(1,720)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	2.12	0.25	2.24
(4,71)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	2.12	0.25	2.24
(4,71)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	2.12	0.25	2.24
(4,71)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	2.12	0.25	2.24
(1,511)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	10	1.93	0.01	1.93
(4,44)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	10	1.93	0.01	1.93
(1,672)	1:15:A:GLY:HA2	1:19:A:SER:HB3	10	1.8	0.48	1.44
(3,609)	1:15:A:GLY:HA2	1:19:A:SER:HB3	10	1.8	0.48	1.44
(1,233)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.8	0.1	1.82
(4,11)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.8	0.1	1.82
(2,601)	1:24:A:PRO:HG2	1:25:A:CYS:H	10	1.7	0.04	1.71
(2,614)	1:10:A:GLN:HA	1:11:A:TRP:HB2	10	1.62	0.03	1.63
(1,451)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	1.6	0.02	1.6
(1,451)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	1.6	0.02	1.6
(4,39)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	1.6	0.02	1.6
(4,39)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	1.6	0.02	1.6
(2,57)	1:3:A:GLU:HG2	1:4:A:CYS:H	10	1.53	0.08	1.56
(2,57)	1:3:A:GLU:HG3	1:4:A:CYS:H	10	1.53	0.08	1.56
(2,694)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	1.47	0.25	1.58
(2,694)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	1.47	0.25	1.58
(2,694)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	1.47	0.25	1.58
(1,534)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	10	1.47	0.05	1.46
(4,49)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	10	1.47	0.05	1.46
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD11	10	1.42	0.0	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD12	10	1.42	0.0	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD13	10	1.42	0.0	1.42
(2,526)	1:4:A:CYS:HA	1:7:A:LEU:HG	10	1.4	0.1	1.42
(1,348)	1:22:A:PRO:HA	1:23:A:PRO:HG2	10	1.36	0.11	1.39
(4,23)	1:22:A:PRO:HA	1:23:A:PRO:HG2	10	1.36	0.11	1.39
(2,223)	1:3:A:GLU:H	1:4:A:CYS:H	10	1.27	0.14	1.27
(1,393)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.26	0.01	1.25
(3,369)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.26	0.01	1.25
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:HA	10	1.25	0.06	1.27
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:HA	10	1.25	0.06	1.27
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:HA	10	1.25	0.06	1.27
(4,47)	1:12:A:LEU:HD21	1:13:A:LYS:HA	10	1.25	0.06	1.27
(4,47)	1:12:A:LEU:HD22	1:13:A:LYS:HA	10	1.25	0.06	1.27
(4,47)	1:12:A:LEU:HD23	1:13:A:LYS:HA	10	1.25	0.06	1.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,533)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	10	1.25	0.11	1.27
(4,48)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	10	1.25	0.11	1.27
(2,646)	1:15:A:GLY:HA2	1:19:A:SER:HB3	10	1.18	0.48	0.82
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	10	1.17	0.22	1.18
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	10	1.17	0.22	1.18
(2,227)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.15	0.1	1.17
(2,423)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	10	1.14	0.05	1.14
(2,423)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	10	1.14	0.05	1.14
(1,748)	1:5:A:VAL:HB	1:9:A:ILE:HG12	10	1.13	0.09	1.17
(4,78)	1:5:A:VAL:HB	1:9:A:ILE:HG12	10	1.13	0.09	1.17
(1,510)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	10	1.1	0.0	1.1
(4,43)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	10	1.1	0.0	1.1
(2,459)	1:14:A:ASP:HB2	1:15:A:GLY:H	10	1.03	0.29	1.12
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	10	1.01	0.03	1.03
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	10	1.01	0.03	1.03
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	10	1.01	0.03	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD11	10	1.01	0.03	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD12	10	1.01	0.03	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD13	10	1.01	0.03	1.03
(2,537)	1:8:A:TYR:HA	1:24:A:PRO:HG2	10	1.01	0.02	1.02
(2,710)	1:9:A:ILE:HA	1:12:A:LEU:HB2	10	1.0	0.01	1.0
(2,573)	1:21:A:ARG:HD3	1:21:A:ARG:HE	10	0.96	0.19	0.92
(2,436)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	0.96	0.02	0.96
(2,436)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	0.96	0.02	0.96
(2,404)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	10	0.95	0.1	0.97
(2,404)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	10	0.95	0.1	0.97
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.94	0.01	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.94	0.01	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.94	0.01	0.94
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	10	0.94	0.12	0.9
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	10	0.94	0.12	0.9
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	10	0.94	0.12	0.9
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	10	0.94	0.12	0.9
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	10	0.94	0.12	0.9
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	10	0.94	0.12	0.9
(1,408)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.93	0.03	0.93
(3,380)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.93	0.03	0.93
(2,538)	1:8:A:TYR:HA	1:24:A:PRO:HG3	10	0.93	0.04	0.94
(1,274)	1:11:A:TRP:H	1:12:A:LEU:HA	10	0.93	0.1	0.92
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.93	0.06	0.92
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.93	0.06	0.92
(4,16)	1:11:A:TRP:H	1:12:A:LEU:HA	10	0.93	0.1	0.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,394)	1:8:A:TYR:HD1	1:12:A:LEU:HA	10	0.88	0.02	0.88
(1,394)	1:8:A:TYR:HD2	1:12:A:LEU:HA	10	0.88	0.02	0.88
(4,25)	1:8:A:TYR:HD1	1:12:A:LEU:HA	10	0.88	0.02	0.88
(4,25)	1:8:A:TYR:HD2	1:12:A:LEU:HA	10	0.88	0.02	0.88
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD11	10	0.88	0.02	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD12	10	0.88	0.02	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD13	10	0.88	0.02	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD21	10	0.88	0.02	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD22	10	0.88	0.02	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD23	10	0.88	0.02	0.89
(2,513)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	10	0.88	0.05	0.88
(1,242)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.88	0.03	0.87
(4,12)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.88	0.03	0.87
(2,392)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	10	0.87	0.08	0.87
(2,392)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	10	0.87	0.08	0.87
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	10	0.86	0.45	1.14
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	10	0.86	0.45	1.14
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	10	0.86	0.45	1.14
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	10	0.86	0.45	1.14
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	10	0.86	0.45	1.14
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	10	0.86	0.45	1.14
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	0.85	0.07	0.87
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	0.85	0.07	0.87
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	0.85	0.07	0.87
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	0.85	0.07	0.87
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	0.85	0.07	0.87
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	0.85	0.07	0.87
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	0.85	0.07	0.87
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	0.85	0.07	0.87
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	0.85	0.07	0.87
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	0.85	0.07	0.87
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	0.85	0.07	0.87
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	0.85	0.07	0.87
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	10	0.84	0.27	0.98
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	10	0.84	0.27	0.98
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	10	0.84	0.27	0.98
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	10	0.84	0.27	0.98
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	10	0.84	0.27	0.98
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	10	0.84	0.27	0.98
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	10	0.84	0.27	0.98
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	10	0.84	0.27	0.98
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	10	0.84	0.27	0.98

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	10	0.84	0.27	0.98
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	10	0.84	0.27	0.98
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	10	0.84	0.27	0.98
(2,689)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	10	0.84	0.04	0.84
(2,689)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	10	0.84	0.04	0.84
(2,689)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	10	0.84	0.04	0.84
(2,560)	1:6:A:ARG:HA	1:6:A:ARG:HD3	10	0.8	0.07	0.78
(1,96)	1:2:A:GLU:HG2	1:5:A:VAL:H	10	0.78	0.23	0.83
(3,91)	1:2:A:GLU:HG2	1:5:A:VAL:H	10	0.78	0.23	0.83
(2,401)	1:11:A:TRP:HZ3	1:23:A:PRO:HB3	10	0.77	0.08	0.78
(2,474)	1:8:A:TYR:HD1	1:25:A:CYS:H	10	0.77	0.11	0.79
(2,474)	1:8:A:TYR:HD2	1:25:A:CYS:H	10	0.77	0.11	0.79
(1,711)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.77	0.31	0.92
(1,711)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.77	0.31	0.92
(1,711)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.77	0.31	0.92
(4,68)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.77	0.31	0.92
(4,68)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.77	0.31	0.92
(4,68)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.77	0.31	0.92
(2,504)	1:14:A:ASP:HB3	1:19:A:SER:HB2	10	0.76	0.32	0.7
(2,636)	1:11:A:TRP:HE3	1:24:A:PRO:HD2	10	0.76	0.04	0.75
(2,611)	1:19:A:SER:HB3	1:19:A:SER:HG	10	0.75	0.03	0.75
(2,477)	1:18:A:SER:H	1:19:A:SER:H	10	0.74	0.39	0.6
(2,379)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	0.74	0.01	0.74
(2,643)	1:8:A:TYR:H	1:10:A:GLN:H	10	0.74	0.05	0.72
(2,357)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	10	0.73	0.12	0.7
(2,472)	1:8:A:TYR:HD1	1:9:A:ILE:H	10	0.73	0.08	0.72
(2,472)	1:8:A:TYR:HD2	1:9:A:ILE:H	10	0.73	0.08	0.72
(2,743)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	0.72	0.02	0.72
(1,252)	1:7:A:LEU:HG	1:25:A:CYS:H	10	0.72	0.26	0.8
(4,13)	1:7:A:LEU:HG	1:25:A:CYS:H	10	0.72	0.26	0.8
(1,397)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.72	0.01	0.72
(3,372)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.72	0.01	0.72
(2,502)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	10	0.72	0.03	0.72
(2,337)	1:22:A:PRO:HA	1:23:A:PRO:HG2	10	0.71	0.11	0.75
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	10	0.7	0.05	0.72
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	10	0.7	0.05	0.72
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	10	0.7	0.05	0.72
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	10	0.7	0.05	0.72
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	10	0.7	0.05	0.72
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	10	0.7	0.05	0.72
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	10	0.7	0.05	0.72
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	10	0.7	0.05	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	10	0.7	0.05	0.72
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	10	0.7	0.05	0.72
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	10	0.7	0.05	0.72
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	10	0.7	0.05	0.72
(1,675)	1:5:A:VAL:HA	1:25:A:CYS:HB3	10	0.7	0.56	0.42
(4,64)	1:5:A:VAL:HA	1:25:A:CYS:HB3	10	0.7	0.56	0.42
(2,496)	1:12:A:LEU:HD21	1:13:A:LYS:HA	10	0.69	0.06	0.7
(2,496)	1:12:A:LEU:HD22	1:13:A:LYS:HA	10	0.69	0.06	0.7
(2,496)	1:12:A:LEU:HD23	1:13:A:LYS:HA	10	0.69	0.06	0.7
(1,545)	1:4:A:CYS:HA	1:7:A:LEU:HB3	10	0.69	0.17	0.68
(4,50)	1:4:A:CYS:HA	1:7:A:LEU:HB3	10	0.69	0.17	0.68
(1,723)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	10	0.69	0.02	0.69
(1,723)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	10	0.69	0.02	0.69
(1,723)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	10	0.69	0.02	0.69
(3,651)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	10	0.69	0.02	0.69
(3,651)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	10	0.69	0.02	0.69
(3,651)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	10	0.69	0.02	0.69
(2,441)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	10	0.68	0.08	0.66
(2,441)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	10	0.68	0.08	0.66
(1,401)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.67	0.01	0.67
(3,375)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.67	0.01	0.67
(2,77)	1:6:A:ARG:HA	1:6:A:ARG:HG2	10	0.67	0.03	0.67
(1,128)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.66	0.01	0.66
(4,6)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.66	0.01	0.66
(2,486)	1:15:A:GLY:H	1:16:A:GLY:H	10	0.66	0.03	0.66
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG21	10	0.65	0.14	0.62
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG22	10	0.65	0.14	0.62
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG23	10	0.65	0.14	0.62
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG21	10	0.65	0.14	0.62
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG22	10	0.65	0.14	0.62
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG23	10	0.65	0.14	0.62
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	10	0.65	0.02	0.64
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	10	0.65	0.02	0.64
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	10	0.65	0.02	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	10	0.65	0.02	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	10	0.65	0.02	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	10	0.65	0.02	0.64
(2,512)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	10	0.64	0.11	0.68
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.64	0.06	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.64	0.06	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.64	0.06	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.64	0.06	0.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.64	0.06	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.64	0.06	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.64	0.06	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.64	0.06	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.64	0.06	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.64	0.06	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.64	0.06	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.64	0.06	0.66
(1,515)	1:5:A:VAL:HG21	1:6:A:ARG:HA	10	0.64	0.17	0.71
(1,515)	1:5:A:VAL:HG22	1:6:A:ARG:HA	10	0.64	0.17	0.71
(1,515)	1:5:A:VAL:HG23	1:6:A:ARG:HA	10	0.64	0.17	0.71
(4,46)	1:5:A:VAL:HG21	1:6:A:ARG:HA	10	0.64	0.17	0.71
(4,46)	1:5:A:VAL:HG22	1:6:A:ARG:HA	10	0.64	0.17	0.71
(4,46)	1:5:A:VAL:HG23	1:6:A:ARG:HA	10	0.64	0.17	0.71
(1,702)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	10	0.63	0.12	0.68
(3,635)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	10	0.63	0.12	0.68
(1,731)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	10	0.63	0.04	0.62
(4,74)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	10	0.63	0.04	0.62
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	0.63	0.0	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	0.63	0.0	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	10	0.63	0.0	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	10	0.63	0.0	0.63
(2,679)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	10	0.62	0.1	0.61
(2,679)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	10	0.62	0.1	0.61
(2,679)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	10	0.62	0.1	0.61
(2,706)	1:7:A:LEU:HG	1:25:A:CYS:HB2	10	0.62	0.2	0.7
(2,275)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.61	0.05	0.6
(2,275)	1:8:A:TYR:HB3	1:9:A:ILE:H	10	0.61	0.05	0.6
(2,572)	1:21:A:ARG:HD2	1:21:A:ARG:HE	10	0.61	0.15	0.56
(2,703)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	10	0.6	0.05	0.62
(1,631)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.6	0.27	0.45
(3,572)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.6	0.27	0.45
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.59	0.01	0.59
(3,230)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.59	0.01	0.59
(2,118)	1:11:A:TRP:HA	1:11:A:TRP:HB2	10	0.59	0.01	0.59
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	10	0.59	0.5	0.34
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	10	0.59	0.5	0.34
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	10	0.59	0.5	0.34
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	10	0.59	0.5	0.34
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	10	0.59	0.5	0.34
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	10	0.59	0.5	0.34
(2,403)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	10	0.59	0.04	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	10	0.59	0.5	0.34
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	10	0.59	0.5	0.34
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	10	0.59	0.5	0.34
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	10	0.59	0.5	0.34
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	10	0.59	0.5	0.34
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	10	0.59	0.5	0.34
(2,42)	1:13:A:LYS:HA	1:13:A:LYS:HD2	10	0.58	0.07	0.6
(2,480)	1:19:A:SER:H	1:20:A:GLY:H	10	0.58	0.21	0.48
(1,617)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.58	0.06	0.6
(1,617)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.58	0.06	0.6
(1,617)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.58	0.06	0.6
(4,59)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.58	0.06	0.6
(4,59)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.58	0.06	0.6
(4,59)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.58	0.06	0.6
(2,722)	1:5:A:VAL:HB	1:9:A:ILE:HG12	10	0.57	0.09	0.62
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB2	10	0.57	0.14	0.54
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB3	10	0.57	0.14	0.54
(1,123)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.56	0.03	0.56
(3,118)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.56	0.03	0.56
(2,628)	1:14:A:ASP:HB3	1:15:A:GLY:H	10	0.55	0.23	0.48
(1,508)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	10	0.55	0.01	0.55
(4,42)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	10	0.55	0.01	0.55
(2,429)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	10	0.55	0.03	0.55
(2,375)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	10	0.55	0.03	0.53
(2,321)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	10	0.55	0.0	0.55
(2,741)	1:2:A:GLU:HA	1:5:A:VAL:H	10	0.54	0.26	0.5
(1,615)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.53	0.04	0.55
(1,615)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.53	0.04	0.55
(1,615)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.53	0.04	0.55
(4,58)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.53	0.04	0.55
(4,58)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.53	0.04	0.55
(4,58)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.53	0.04	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD11	10	0.53	0.02	0.54
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD12	10	0.53	0.02	0.54
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD13	10	0.53	0.02	0.54
(2,387)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	0.53	0.01	0.52
(1,658)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.53	0.05	0.54
(1,658)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.53	0.05	0.54
(3,596)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.53	0.05	0.54
(3,596)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.53	0.05	0.54
(2,245)	1:24:A:PRO:HB2	1:25:A:CYS:H	10	0.52	0.12	0.54
(2,586)	1:12:A:LEU:H	1:12:A:LEU:HB2	10	0.52	0.01	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,460)	1:24:A:PRO:HD2	1:25:A:CYS:H	10	0.52	0.1	0.52
(2,289)	1:12:A:LEU:HA	1:12:A:LEU:HG	10	0.51	0.02	0.51
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	10	0.5	0.14	0.54
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	10	0.5	0.14	0.54
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	10	0.5	0.14	0.54
(2,701)	1:8:A:TYR:HB2	1:9:A:ILE:HG12	10	0.5	0.08	0.48
(2,701)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	10	0.5	0.08	0.48
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG2	10	0.49	0.25	0.38
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG3	10	0.49	0.25	0.38
(2,510)	1:8:A:TYR:HA	1:24:A:PRO:HD2	10	0.48	0.05	0.49
(2,563)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	10	0.48	0.03	0.48
(1,439)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	0.48	0.08	0.42
(1,439)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	0.48	0.08	0.42
(4,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	0.48	0.08	0.42
(4,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	0.48	0.08	0.42
(2,215)	1:21:A:ARG:HA	1:22:A:PRO:HD3	10	0.48	0.05	0.48
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD21	10	0.48	0.04	0.48
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD22	10	0.48	0.04	0.48
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD23	10	0.48	0.04	0.48
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG2	10	0.47	0.04	0.47
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG3	10	0.47	0.04	0.47
(2,449)	1:8:A:TYR:HD1	1:12:A:LEU:HB3	10	0.46	0.02	0.46
(2,449)	1:8:A:TYR:HD2	1:12:A:LEU:HB3	10	0.46	0.02	0.46
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	10	0.45	0.08	0.48
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	10	0.45	0.08	0.48
(1,56)	1:2:A:GLU:HB3	1:3:A:GLU:H	10	0.45	0.02	0.46
(3,54)	1:2:A:GLU:HB3	1:3:A:GLU:H	10	0.45	0.02	0.46
(2,484)	1:4:A:CYS:H	1:5:A:VAL:H	10	0.45	0.09	0.48
(2,154)	1:25:A:CYS:H	1:25:A:CYS:HB2	10	0.45	0.14	0.42
(2,68)	1:10:A:GLN:H	1:10:A:GLN:HB2	10	0.45	0.04	0.44
(1,743)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	10	0.44	0.28	0.32
(4,76)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	10	0.44	0.28	0.32
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG21	10	0.43	0.19	0.38
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG22	10	0.43	0.19	0.38
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG23	10	0.43	0.19	0.38
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG21	10	0.43	0.19	0.38
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG22	10	0.43	0.19	0.38
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG23	10	0.43	0.19	0.38
(1,413)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.43	0.06	0.45
(1,413)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.43	0.06	0.45
(2,618)	1:6:A:ARG:HA	1:8:A:TYR:H	10	0.43	0.04	0.44
(3,383)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.43	0.06	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,383)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.43	0.06	0.45
(2,142)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.43	0.01	0.43
(2,136)	1:18:A:SER:H	1:18:A:SER:HA	10	0.43	0.19	0.37
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	10	0.41	0.01	0.41
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	10	0.41	0.01	0.41
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	10	0.41	0.01	0.41
(1,450)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.41	0.02	0.41
(4,38)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.41	0.02	0.41
(2,612)	1:19:A:SER:HB2	1:19:A:SER:HG	10	0.41	0.05	0.39
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.4	0.1	0.36
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.4	0.1	0.36
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.4	0.1	0.36
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.4	0.1	0.36
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.4	0.1	0.36
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.4	0.1	0.36
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.4	0.1	0.36
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.4	0.1	0.36
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.4	0.1	0.36
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.4	0.1	0.36
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.4	0.1	0.36
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.4	0.1	0.36
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	10	0.4	0.1	0.37
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	10	0.4	0.1	0.37
(2,678)	1:12:A:LEU:HB2	1:13:A:LYS:HD2	10	0.4	0.09	0.36
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	10	0.4	0.02	0.4
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	10	0.4	0.02	0.4
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	10	0.4	0.02	0.4
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	10	0.4	0.02	0.4
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	10	0.4	0.02	0.4
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	10	0.4	0.02	0.4
(2,445)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	10	0.4	0.09	0.4
(2,445)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	10	0.4	0.09	0.4
(1,60)	1:2:A:GLU:HB3	1:4:A:CYS:H	10	0.4	0.16	0.36
(3,58)	1:2:A:GLU:HB3	1:4:A:CYS:H	10	0.4	0.16	0.36
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	10	0.4	0.03	0.4
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	10	0.4	0.03	0.4
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	10	0.4	0.03	0.4
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD11	10	0.4	0.03	0.4
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD12	10	0.4	0.03	0.4
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD13	10	0.4	0.03	0.4
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.39	0.02	0.39
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	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)
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.39	0.02	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	10	0.39	0.02	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	10	0.39	0.02	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	10	0.39	0.02	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.39	0.02	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.39	0.02	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.39	0.02	0.39
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	10	0.39	0.02	0.39
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	10	0.39	0.02	0.39
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	10	0.39	0.02	0.39
(2,355)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	10	0.39	0.01	0.39
(2,557)	1:23:A:PRO:HA	1:24:A:PRO:HD2	10	0.38	0.02	0.39
(1,463)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	10	0.38	0.02	0.4
(3,424)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	10	0.38	0.02	0.4
(1,462)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	10	0.38	0.07	0.34
(1,462)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	10	0.38	0.07	0.34
(3,423)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	10	0.38	0.07	0.34
(3,423)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	10	0.38	0.07	0.34
(1,410)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	10	0.38	0.06	0.38
(1,410)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	10	0.38	0.06	0.38
(3,381)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	10	0.38	0.06	0.38
(3,381)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	10	0.38	0.06	0.38
(1,575)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	10	0.38	0.04	0.38
(3,519)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	10	0.38	0.04	0.38
(2,600)	1:11:A:TRP:H	1:11:A:TRP:HB3	10	0.37	0.03	0.38
(2,109)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	10	0.37	0.1	0.38
(2,133)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	10	0.37	0.0	0.37
(2,350)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.36	0.01	0.36
(2,319)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.36	0.01	0.36
(2,278)	1:7:A:LEU:HA	1:7:A:LEU:HB3	10	0.36	0.03	0.35
(2,317)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.35	0.01	0.35
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	10	0.35	0.08	0.38
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	10	0.35	0.08	0.38
(1,271)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.35	0.02	0.34
(4,15)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.35	0.02	0.34
(1,749)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	10	0.34	0.07	0.38
(4,79)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	10	0.34	0.07	0.38
(2,125)	1:9:A:ILE:HA	1:9:A:ILE:HG12	10	0.34	0.04	0.36
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	10	0.34	0.04	0.33
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	10	0.34	0.04	0.33
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	10	0.34	0.04	0.33
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	10	0.34	0.04	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	10	0.34	0.04	0.33
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	10	0.34	0.04	0.33
(2,268)	1:11:A:TRP:H	1:12:A:LEU:HA	10	0.34	0.09	0.34
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	10	0.34	0.06	0.38
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	10	0.34	0.06	0.38
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	10	0.34	0.06	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	10	0.34	0.06	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	10	0.34	0.06	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	10	0.34	0.06	0.38
(1,75)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.34	0.04	0.34
(4,3)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.34	0.04	0.34
(1,730)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	10	0.34	0.03	0.34
(3,657)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	10	0.34	0.03	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.34	0.01	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.34	0.01	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.34	0.01	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.34	0.01	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.34	0.01	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.34	0.01	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.34	0.01	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.34	0.01	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.34	0.01	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.34	0.01	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.34	0.01	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.34	0.01	0.34
(2,120)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.33	0.0	0.33
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	10	0.33	0.05	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	10	0.33	0.05	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	10	0.33	0.05	0.36
(2,36)	1:12:A:LEU:HB2	1:13:A:LYS:H	10	0.33	0.02	0.32
(1,622)	1:24:A:PRO:HG2	1:25:A:CYS:H	10	0.33	0.04	0.33
(3,563)	1:24:A:PRO:HG2	1:25:A:CYS:H	10	0.33	0.04	0.33
(2,566)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.32	0.02	0.32
(2,393)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.32	0.03	0.32
(2,426)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	10	0.32	0.11	0.32
(2,426)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	10	0.32	0.11	0.32
(2,320)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.31	0.0	0.31
(1,605)	1:8:A:TYR:H	1:9:A:ILE:HB	10	0.31	0.02	0.31
(4,57)	1:8:A:TYR:H	1:9:A:ILE:HB	10	0.31	0.02	0.31
(1,278)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	10	0.3	0.01	0.3
(4,17)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	10	0.3	0.01	0.3
(2,200)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.3	0.02	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,353)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.29	0.01	0.3
(2,139)	1:18:A:SER:HB2	1:18:A:SER:HB3	10	0.29	0.0	0.29
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.28	0.01	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.28	0.01	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.28	0.01	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.28	0.01	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.28	0.01	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.28	0.01	0.28
(2,204)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.28	0.01	0.28
(2,582)	1:7:A:LEU:HG	1:8:A:TYR:H	10	0.27	0.09	0.24
(2,222)	1:8:A:TYR:H	1:9:A:ILE:H	10	0.27	0.02	0.28
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	10	0.27	0.02	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	10	0.27	0.02	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	10	0.27	0.02	0.26
(2,286)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	10	0.27	0.0	0.27
(2,73)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.27	0.01	0.27
(2,328)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.27	0.01	0.27
(1,262)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.26	0.04	0.26
(4,14)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.26	0.04	0.26
(2,212)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.26	0.0	0.26
(1,681)	1:6:A:ARG:HA	1:9:A:ILE:HG13	10	0.26	0.03	0.25
(2,311)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.26	0.0	0.26
(4,66)	1:6:A:ARG:HA	1:9:A:ILE:HG13	10	0.26	0.03	0.25
(2,376)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	10	0.26	0.06	0.26
(1,585)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	10	0.26	0.03	0.26
(3,529)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	10	0.26	0.03	0.26
(1,192)	1:24:A:PRO:HA	1:25:A:CYS:H	10	0.25	0.01	0.24
(4,9)	1:24:A:PRO:HA	1:25:A:CYS:H	10	0.25	0.01	0.24
(2,8)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.25	0.01	0.24
(2,24)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.25	0.01	0.24
(2,277)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.24	0.0	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB2	10	0.24	0.0	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB3	10	0.24	0.0	0.24
(1,663)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	0.23	0.05	0.24
(4,63)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	0.23	0.05	0.24
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.23	0.03	0.22
(2,313)	1:19:A:SER:HB2	1:19:A:SER:HB3	10	0.23	0.01	0.22
(2,516)	1:2:A:GLU:HA	1:2:A:GLU:HB3	10	0.23	0.02	0.22
(2,515)	1:2:A:GLU:HA	1:2:A:GLU:HB2	10	0.22	0.03	0.22
(2,294)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.22	0.0	0.22
(2,294)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.22	0.0	0.22
(2,294)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.22	0.0	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,556)	1:23:A:PRO:HA	1:24:A:PRO:HD3	10	0.21	0.03	0.2
(2,88)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	10	0.21	0.0	0.21
(1,357)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.21	0.01	0.21
(3,334)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.21	0.01	0.21
(1,291)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.21	0.03	0.21
(4,19)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.21	0.03	0.21
(2,290)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.2	0.0	0.2
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	10	0.2	0.09	0.16
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	10	0.2	0.09	0.16
(2,207)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.2	0.01	0.2
(2,282)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.2	0.0	0.2
(1,643)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.2	0.03	0.21
(4,62)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.2	0.03	0.21
(1,506)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.2	0.0	0.2
(4,41)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.2	0.0	0.2
(1,738)	1:10:A:GLN:HA	1:13:A:LYS:HD2	10	0.2	0.06	0.18
(4,75)	1:10:A:GLN:HA	1:13:A:LYS:HD2	10	0.2	0.06	0.18
(2,65)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	10	0.2	0.0	0.2
(2,569)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	10	0.19	0.02	0.19
(1,504)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	10	0.19	0.0	0.19
(4,40)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	10	0.19	0.0	0.19
(2,334)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.19	0.03	0.19
(1,280)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	10	0.18	0.01	0.18
(3,263)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	10	0.18	0.01	0.18
(2,201)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	10	0.18	0.0	0.18
(1,81)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	10	0.18	0.01	0.18
(4,4)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	10	0.18	0.01	0.18
(2,152)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	10	0.17	0.05	0.16
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.17	0.01	0.18
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.17	0.01	0.18
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.17	0.01	0.18
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.17	0.01	0.18
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.17	0.01	0.18
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.17	0.01	0.18
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.17	0.01	0.18
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.17	0.01	0.18
(2,71)	1:5:A:VAL:H	1:5:A:VAL:HB	10	0.17	0.06	0.15
(2,359)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	10	0.17	0.01	0.17
(1,566)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	10	0.17	0.02	0.16
(3,513)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	10	0.17	0.02	0.16
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG21	10	0.17	0.03	0.17
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG22	10	0.17	0.03	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG23	10	0.17	0.03	0.17
(1,359)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	0.16	0.02	0.17
(3,336)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	0.16	0.02	0.17
(2,233)	1:9:A:ILE:H	1:9:A:ILE:HG13	10	0.16	0.04	0.16
(2,745)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	10	0.16	0.02	0.16
(2,354)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	10	0.16	0.01	0.16
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD11	10	0.16	0.02	0.16
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD12	10	0.16	0.02	0.16
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD13	10	0.16	0.02	0.16
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	10	0.16	0.02	0.16
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	10	0.16	0.02	0.16
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	10	0.16	0.02	0.16
(1,318)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	10	0.16	0.02	0.16
(4,22)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	10	0.16	0.02	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG2	10	0.16	0.0	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG3	10	0.16	0.0	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG2	10	0.16	0.0	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG3	10	0.16	0.0	0.16
(1,270)	1:16:A:GLY:H	1:17:A:PRO:HD2	10	0.15	0.02	0.15
(3,256)	1:16:A:GLY:H	1:17:A:PRO:HD2	10	0.15	0.02	0.15
(2,345)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	10	0.15	0.0	0.15
(2,518)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	10	0.15	0.01	0.15
(1,213)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	10	0.15	0.08	0.13
(3,203)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	10	0.15	0.08	0.13
(2,295)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.15	0.0	0.15
(2,295)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.15	0.0	0.15
(2,295)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.15	0.0	0.15
(2,329)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.15	0.01	0.15
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.14	0.0	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.14	0.0	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.14	0.0	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.14	0.0	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.14	0.0	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.14	0.0	0.14
(2,300)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.14	0.01	0.14
(1,455)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	0.14	0.01	0.15
(2,304)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.14	0.01	0.14
(3,416)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	0.14	0.01	0.15
(2,351)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	10	0.13	0.0	0.13
(2,306)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.11	0.0	0.11
(1,95)	1:2:A:GLU:HG2	1:6:A:ARG:H	9	1.15	0.2	1.08
(3,90)	1:2:A:GLU:HG2	1:6:A:ARG:H	9	1.15	0.2	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,252)	1:10:A:GLN:HA	1:10:A:GLN:HE21	9	1.11	0.07	1.14
(2,739)	1:13:A:LYS:H	1:14:A:ASP:HB3	9	0.78	0.05	0.79
(2,155)	1:25:A:CYS:H	1:25:A:CYS:HB3	9	0.64	0.12	0.57
(2,94)	1:2:A:GLU:HG2	1:6:A:ARG:H	9	0.59	0.2	0.52
(2,184)	1:19:A:SER:HG	1:21:A:ARG:H	9	0.57	0.38	0.51
(2,521)	1:14:A:ASP:HB2	1:16:A:GLY:H	9	0.5	0.07	0.51
(1,193)	1:18:A:SER:H	1:19:A:SER:HB2	9	0.5	0.43	0.33
(3,184)	1:18:A:SER:H	1:19:A:SER:HB2	9	0.5	0.43	0.33
(2,465)	1:10:A:GLN:HA	1:10:A:GLN:HE22	9	0.48	0.05	0.49
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD11	9	0.47	0.25	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD12	9	0.47	0.25	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD13	9	0.47	0.25	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD21	9	0.47	0.25	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD22	9	0.47	0.25	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD23	9	0.47	0.25	0.36
(2,536)	1:22:A:PRO:HB2	1:23:A:PRO:HD2	9	0.45	0.03	0.45
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	9	0.44	0.09	0.4
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	9	0.44	0.09	0.4
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	9	0.44	0.09	0.4
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	9	0.44	0.09	0.4
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	9	0.44	0.09	0.4
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	9	0.44	0.09	0.4
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	9	0.43	0.15	0.4
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	9	0.43	0.15	0.4
(1,726)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(1,726)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(1,726)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(1,726)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(1,726)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(1,726)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(3,653)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(3,653)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(3,653)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(3,653)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(3,653)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(3,653)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	9	0.41	0.18	0.28
(2,625)	1:19:A:SER:HG	1:20:A:GLY:H	9	0.39	0.15	0.34
(2,95)	1:2:A:GLU:HG2	1:5:A:VAL:H	9	0.36	0.09	0.36
(2,363)	1:11:A:TRP:HZ2	1:22:A:PRO:HA	9	0.35	0.04	0.35
(2,193)	1:11:A:TRP:HE1	1:22:A:PRO:HA	9	0.3	0.06	0.29
(2,402)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	9	0.28	0.1	0.29
(2,402)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	9	0.28	0.1	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,608)	1:6:A:ARG:HA	1:9:A:ILE:HB	9	0.25	0.04	0.26
(2,737)	1:12:A:LEU:HB3	1:14:A:ASP:H	9	0.23	0.07	0.27
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	9	0.23	0.04	0.24
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	9	0.23	0.04	0.24
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	9	0.23	0.04	0.24
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	9	0.23	0.04	0.24
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	9	0.23	0.04	0.24
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	9	0.23	0.04	0.24
(2,522)	1:3:A:GLU:HG2	1:4:A:CYS:HA	9	0.19	0.06	0.18
(2,522)	1:3:A:GLU:HG3	1:4:A:CYS:HA	9	0.19	0.06	0.18
(1,86)	1:14:A:ASP:H	1:14:A:ASP:HB3	9	0.19	0.02	0.19
(4,5)	1:14:A:ASP:H	1:14:A:ASP:HB3	9	0.19	0.02	0.19
(2,517)	1:2:A:GLU:HA	1:3:A:GLU:H	9	0.18	0.02	0.18
(1,519)	1:8:A:TYR:HA	1:11:A:TRP:HB2	9	0.18	0.05	0.17
(3,472)	1:8:A:TYR:HA	1:11:A:TRP:HB2	9	0.18	0.05	0.17
(1,728)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	9	0.18	0.04	0.18
(3,655)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	9	0.18	0.04	0.18
(1,220)	1:21:A:ARG:HA	1:22:A:PRO:HD2	9	0.17	0.03	0.18
(3,210)	1:21:A:ARG:HA	1:22:A:PRO:HD2	9	0.17	0.03	0.18
(1,232)	1:11:A:TRP:H	1:24:A:PRO:HG2	9	0.14	0.04	0.14
(3,222)	1:11:A:TRP:H	1:24:A:PRO:HG2	9	0.14	0.04	0.14
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	9	0.12	0.01	0.13
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	9	0.12	0.01	0.13
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	9	0.12	0.01	0.13
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	9	0.12	0.01	0.13
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	9	0.12	0.01	0.13
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	9	0.12	0.01	0.13
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB2	9	0.11	0.0	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB3	9	0.11	0.0	0.11
(1,682)	1:17:A:PRO:HB2	1:18:A:SER:HB3	8	1.25	0.16	1.31
(3,616)	1:17:A:PRO:HB2	1:18:A:SER:HB3	8	1.25	0.16	1.31
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG2	8	1.02	0.07	1.02
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG3	8	1.02	0.07	1.02
(1,697)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	8	0.8	0.1	0.79
(1,697)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	8	0.8	0.1	0.79
(1,697)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	8	0.8	0.1	0.79
(3,630)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	8	0.8	0.1	0.79
(3,630)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	8	0.8	0.1	0.79
(3,630)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	8	0.8	0.1	0.79
(2,656)	1:17:A:PRO:HB2	1:18:A:SER:HB3	8	0.65	0.16	0.7
(2,579)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	8	0.63	0.11	0.6
(2,466)	1:17:A:PRO:HA	1:18:A:SER:H	8	0.58	0.44	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,433)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	8	0.44	0.05	0.45
(2,99)	1:21:A:ARG:HA	1:21:A:ARG:HB3	8	0.4	0.03	0.41
(1,632)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	8	0.33	0.11	0.34
(3,573)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	8	0.33	0.11	0.34
(1,52)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	8	0.29	0.03	0.29
(1,52)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	8	0.29	0.03	0.29
(3,50)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	8	0.29	0.03	0.29
(3,50)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	8	0.29	0.03	0.29
(2,102)	1:21:A:ARG:H	1:21:A:ARG:HD2	8	0.28	0.07	0.26
(2,671)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	8	0.27	0.09	0.26
(2,671)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	8	0.27	0.09	0.26
(2,671)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	8	0.27	0.09	0.26
(2,185)	1:20:A:GLY:HA3	1:21:A:ARG:H	8	0.25	0.11	0.24
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	8	0.24	0.07	0.22
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	8	0.24	0.07	0.22
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	8	0.24	0.07	0.22
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	8	0.24	0.07	0.22
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	8	0.24	0.07	0.22
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	8	0.24	0.07	0.22
(2,307)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	8	0.23	0.05	0.25
(2,61)	1:4:A:CYS:H	1:4:A:CYS:HB3	8	0.19	0.09	0.15
(2,494)	1:5:A:VAL:HG21	1:6:A:ARG:HA	8	0.18	0.03	0.17
(2,494)	1:5:A:VAL:HG22	1:6:A:ARG:HA	8	0.18	0.03	0.17
(2,494)	1:5:A:VAL:HG23	1:6:A:ARG:HA	8	0.18	0.03	0.17
(2,452)	1:11:A:TRP:HE3	1:23:A:PRO:HA	8	0.15	0.04	0.15
(2,744)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	8	0.14	0.01	0.14
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH21	7	1.16	0.96	0.51
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH22	7	1.16	0.96	0.51
(2,575)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	7	1.02	0.28	1.03
(1,745)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	7	0.96	0.14	0.89
(1,745)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	7	0.96	0.14	0.89
(3,669)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	7	0.96	0.14	0.89
(3,669)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	7	0.96	0.14	0.89
(2,60)	1:4:A:CYS:H	1:4:A:CYS:HB2	7	0.59	0.12	0.56
(2,648)	1:11:A:TRP:HA	1:21:A:ARG:HD2	7	0.57	0.23	0.6
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	7	0.55	0.15	0.56
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	7	0.55	0.15	0.56
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	7	0.55	0.15	0.56
(2,462)	1:4:A:CYS:HB3	1:5:A:VAL:H	7	0.5	0.11	0.57
(2,719)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	7	0.44	0.14	0.37
(2,719)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	7	0.44	0.14	0.37
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	7	0.36	0.06	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	7	0.36	0.06	0.38
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	7	0.36	0.06	0.38
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	7	0.36	0.06	0.38
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	7	0.36	0.06	0.38
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	7	0.36	0.06	0.38
(2,529)	1:1:A:GLU:HA	1:1:A:GLU:HB3	7	0.34	0.03	0.34
(2,685)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	7	0.32	0.06	0.32
(2,685)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	7	0.32	0.06	0.32
(2,685)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	7	0.32	0.06	0.32
(2,438)	1:8:A:TYR:HE1	1:23:A:PRO:HG3	7	0.31	0.07	0.33
(2,438)	1:8:A:TYR:HE2	1:23:A:PRO:HG3	7	0.31	0.07	0.33
(2,244)	1:2:A:GLU:HB2	1:5:A:VAL:H	7	0.22	0.06	0.2
(2,680)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	7	0.2	0.05	0.2
(2,680)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	7	0.2	0.05	0.2
(2,680)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	7	0.2	0.05	0.2
(2,394)	1:8:A:TYR:HE1	1:24:A:PRO:HD2	7	0.17	0.05	0.16
(2,394)	1:8:A:TYR:HE2	1:24:A:PRO:HD2	7	0.17	0.05	0.16
(1,546)	1:4:A:CYS:HA	1:24:A:PRO:HB2	7	0.17	0.02	0.17
(3,496)	1:4:A:CYS:HA	1:24:A:PRO:HB2	7	0.17	0.02	0.17
(2,138)	1:18:A:SER:HA	1:18:A:SER:HB2	7	0.16	0.03	0.15
(2,576)	1:6:A:ARG:H	1:8:A:TYR:H	7	0.16	0.03	0.14
(1,716)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	7	0.15	0.03	0.14
(1,716)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	7	0.15	0.03	0.14
(1,716)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	7	0.15	0.03	0.14
(3,647)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	7	0.15	0.03	0.14
(3,647)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	7	0.15	0.03	0.14
(3,647)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	7	0.15	0.03	0.14
(2,507)	1:11:A:TRP:HA	1:14:A:ASP:HB2	7	0.14	0.03	0.13
(1,750)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	6	1.29	0.01	1.29
(3,671)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	6	1.29	0.01	1.29
(2,724)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	6	0.68	0.01	0.68
(2,528)	1:1:A:GLU:HA	1:1:A:GLU:HB2	6	0.48	0.03	0.46
(2,360)	1:11:A:TRP:HD1	1:19:A:SER:HG	6	0.44	0.24	0.4
(2,135)	1:18:A:SER:H	1:18:A:SER:HB3	6	0.4	0.22	0.38
(2,166)	1:19:A:SER:H	1:19:A:SER:HB3	6	0.38	0.13	0.44
(2,654)	1:3:A:GLU:HA	1:6:A:ARG:HB2	6	0.38	0.14	0.4
(2,183)	1:19:A:SER:H	1:19:A:SER:HG	6	0.32	0.07	0.33
(2,246)	1:7:A:LEU:HG	1:25:A:CYS:H	6	0.31	0.11	0.3
(2,511)	1:14:A:ASP:HB2	1:19:A:SER:HB2	6	0.26	0.15	0.22
(2,495)	1:5:A:VAL:HG11	1:6:A:ARG:HA	6	0.21	0.14	0.12
(2,495)	1:5:A:VAL:HG12	1:6:A:ARG:HA	6	0.21	0.14	0.12
(2,495)	1:5:A:VAL:HG13	1:6:A:ARG:HA	6	0.21	0.14	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,154)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	6	0.2	0.01	0.2
(4,7)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	6	0.2	0.01	0.2
(1,443)	1:23:A:PRO:HB2	1:25:A:CYS:H	6	0.18	0.06	0.16
(4,37)	1:23:A:PRO:HB2	1:25:A:CYS:H	6	0.18	0.06	0.16
(1,514)	1:4:A:CYS:HA	1:7:A:LEU:HB2	6	0.16	0.06	0.13
(4,45)	1:4:A:CYS:HA	1:7:A:LEU:HB2	6	0.16	0.06	0.13
(2,231)	1:7:A:LEU:H	1:7:A:LEU:HG	6	0.14	0.03	0.14
(1,98)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.14	0.02	0.13
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	6	0.14	0.01	0.14
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	6	0.14	0.01	0.14
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	6	0.14	0.01	0.14
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	6	0.14	0.01	0.14
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	6	0.14	0.01	0.14
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	6	0.14	0.01	0.14
(3,93)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.14	0.02	0.13
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG21	6	0.13	0.03	0.12
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG22	6	0.13	0.03	0.12
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG23	6	0.13	0.03	0.12
(2,92)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	6	0.13	0.01	0.14
(1,659)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	6	0.12	0.02	0.11
(1,659)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	6	0.12	0.02	0.11
(3,597)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	6	0.12	0.02	0.11
(3,597)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	6	0.12	0.02	0.11
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH21	5	1.42	0.74	1.76
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH22	5	1.42	0.74	1.76
(2,243)	1:17:A:PRO:HG2	1:18:A:SER:H	5	0.79	0.19	0.79
(2,242)	1:17:A:PRO:HB2	1:18:A:SER:H	5	0.65	0.39	0.64
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	5	0.5	0.16	0.56
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	5	0.5	0.16	0.56
(2,167)	1:19:A:SER:HA	1:19:A:SER:HB2	5	0.2	0.03	0.2
(2,399)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	5	0.18	0.05	0.2
(1,70)	1:10:A:GLN:H	1:10:A:GLN:HB3	5	0.17	0.04	0.18
(3,68)	1:10:A:GLN:H	1:10:A:GLN:HB3	5	0.17	0.04	0.18
(2,675)	1:12:A:LEU:HB3	1:13:A:LYS:HD2	5	0.17	0.06	0.14
(2,425)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	5	0.16	0.04	0.16
(2,425)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	5	0.16	0.04	0.16
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	5	0.15	0.04	0.18
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	5	0.15	0.04	0.18
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	5	0.15	0.04	0.18
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	5	0.15	0.04	0.18
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	5	0.15	0.04	0.18
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	5	0.15	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,670)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	5	0.15	0.02	0.14
(1,670)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	5	0.15	0.02	0.14
(3,607)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	5	0.15	0.02	0.14
(3,607)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	5	0.15	0.02	0.14
(1,686)	1:7:A:LEU:HD11	1:25:A:CYS:HA	5	0.13	0.05	0.11
(1,686)	1:7:A:LEU:HD12	1:25:A:CYS:HA	5	0.13	0.05	0.11
(1,686)	1:7:A:LEU:HD13	1:25:A:CYS:HA	5	0.13	0.05	0.11
(1,686)	1:7:A:LEU:HD21	1:25:A:CYS:HA	5	0.13	0.05	0.11
(1,686)	1:7:A:LEU:HD22	1:25:A:CYS:HA	5	0.13	0.05	0.11
(1,686)	1:7:A:LEU:HD23	1:25:A:CYS:HA	5	0.13	0.05	0.11
(3,620)	1:7:A:LEU:HD11	1:25:A:CYS:HA	5	0.13	0.05	0.11
(3,620)	1:7:A:LEU:HD12	1:25:A:CYS:HA	5	0.13	0.05	0.11
(3,620)	1:7:A:LEU:HD13	1:25:A:CYS:HA	5	0.13	0.05	0.11
(3,620)	1:7:A:LEU:HD21	1:25:A:CYS:HA	5	0.13	0.05	0.11
(3,620)	1:7:A:LEU:HD22	1:25:A:CYS:HA	5	0.13	0.05	0.11
(3,620)	1:7:A:LEU:HD23	1:25:A:CYS:HA	5	0.13	0.05	0.11
(2,84)	1:14:A:ASP:H	1:14:A:ASP:HB2	5	0.12	0.01	0.12
(1,310)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	5	0.12	0.01	0.12
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB2	5	0.12	0.02	0.11
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB3	5	0.12	0.02	0.11
(3,289)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	5	0.12	0.01	0.12
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB2	5	0.12	0.02	0.11
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB3	5	0.12	0.02	0.11
(2,574)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	4	1.13	0.2	1.08
(1,93)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	4	0.55	0.0	0.55
(3,88)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	4	0.55	0.0	0.55
(2,91)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	4	0.54	0.01	0.54
(2,134)	1:18:A:SER:H	1:18:A:SER:HB2	4	0.5	0.18	0.45
(2,742)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	4	0.37	0.27	0.37
(1,469)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	4	0.35	0.0	0.35
(3,430)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	4	0.35	0.0	0.35
(2,145)	1:10:A:GLN:HA	1:10:A:GLN:HG2	4	0.32	0.05	0.31
(2,229)	1:10:A:GLN:HB3	1:11:A:TRP:H	4	0.3	0.06	0.31
(1,263)	1:19:A:SER:HB2	1:21:A:ARG:H	4	0.28	0.18	0.2
(3,249)	1:19:A:SER:HB2	1:21:A:ARG:H	4	0.28	0.18	0.2
(2,457)	1:11:A:TRP:HH2	1:17:A:PRO:HB3	4	0.24	0.1	0.23
(2,146)	1:10:A:GLN:HA	1:10:A:GLN:HG3	4	0.23	0.07	0.24
(2,182)	1:18:A:SER:HA	1:19:A:SER:H	4	0.2	0.03	0.2
(2,713)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	4	0.19	0.05	0.2
(2,713)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	4	0.19	0.05	0.2
(2,362)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	4	0.18	0.06	0.16
(2,644)	1:8:A:TYR:HE1	1:11:A:TRP:HZ3	4	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,644)	1:8:A:TYR:HE2	1:11:A:TRP:HZ3	4	0.16	0.03	0.16
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	4	0.12	0.01	0.12
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	4	0.12	0.01	0.12
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	4	0.12	0.01	0.12
(1,73)	1:5:A:VAL:HB	1:6:A:ARG:H	4	0.12	0.01	0.12
(3,71)	1:5:A:VAL:HB	1:6:A:ARG:H	4	0.12	0.01	0.12
(2,505)	1:4:A:CYS:HB2	1:25:A:CYS:HB2	3	1.35	0.1	1.41
(2,649)	1:5:A:VAL:HA	1:25:A:CYS:HB3	3	0.83	0.44	0.68
(1,630)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	3	0.66	0.06	0.7
(3,571)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	3	0.66	0.06	0.7
(2,192)	1:11:A:TRP:HE1	1:19:A:SER:HG	3	0.41	0.2	0.54
(2,527)	1:1:A:GLU:HA	1:1:A:GLU:HG2	3	0.4	0.02	0.39
(2,527)	1:1:A:GLU:HA	1:1:A:GLU:HG3	3	0.4	0.02	0.39
(2,610)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	0.34	0.15	0.25
(2,467)	1:18:A:SER:HA	1:20:A:GLY:H	3	0.28	0.11	0.34
(1,540)	1:10:A:GLN:HG3	1:11:A:TRP:H	3	0.27	0.05	0.27
(3,491)	1:10:A:GLN:HG3	1:11:A:TRP:H	3	0.27	0.05	0.27
(2,524)	1:4:A:CYS:HA	1:7:A:LEU:HB3	3	0.26	0.08	0.22
(2,598)	1:21:A:ARG:HB2	1:21:A:ARG:HE	3	0.25	0.06	0.29
(2,64)	1:4:A:CYS:HA	1:4:A:CYS:HB2	3	0.25	0.03	0.26
(2,647)	1:11:A:TRP:HA	1:21:A:ARG:HD3	3	0.23	0.17	0.12
(2,683)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	3	0.2	0.08	0.17
(2,683)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	3	0.2	0.08	0.17
(2,683)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	3	0.2	0.08	0.17
(2,110)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	3	0.2	0.03	0.21
(2,218)	1:13:A:LYS:H	1:13:A:LYS:HB2	3	0.14	0.01	0.14
(2,218)	1:13:A:LYS:H	1:13:A:LYS:HB3	3	0.14	0.01	0.14
(2,131)	1:20:A:GLY:H	1:20:A:GLY:HA2	3	0.14	0.02	0.14
(1,68)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.13	0.01	0.12
(3,66)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.13	0.01	0.12
(1,458)	1:8:A:TYR:HE1	1:12:A:LEU:HG	3	0.12	0.02	0.11
(1,458)	1:8:A:TYR:HE2	1:12:A:LEU:HG	3	0.12	0.02	0.11
(2,263)	1:9:A:ILE:HA	1:12:A:LEU:H	3	0.12	0.02	0.11
(3,419)	1:8:A:TYR:HE1	1:12:A:LEU:HG	3	0.12	0.02	0.11
(3,419)	1:8:A:TYR:HE2	1:12:A:LEU:HG	3	0.12	0.02	0.11
(1,11)	1:12:A:LEU:HD21	1:13:A:LYS:H	3	0.11	0.0	0.11
(1,11)	1:12:A:LEU:HD22	1:13:A:LYS:H	3	0.11	0.0	0.11
(1,11)	1:12:A:LEU:HD23	1:13:A:LYS:H	3	0.11	0.0	0.11
(1,27)	1:12:A:LEU:HD21	1:13:A:LYS:H	3	0.11	0.0	0.11
(1,27)	1:12:A:LEU:HD22	1:13:A:LYS:H	3	0.11	0.0	0.11
(1,27)	1:12:A:LEU:HD23	1:13:A:LYS:H	3	0.11	0.0	0.11
(1,177)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	3	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,177)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	3	0.11	0.0	0.11
(1,177)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	3	0.11	0.0	0.11
(3,10)	1:12:A:LEU:HD21	1:13:A:LYS:H	3	0.11	0.0	0.11
(3,10)	1:12:A:LEU:HD22	1:13:A:LYS:H	3	0.11	0.0	0.11
(3,10)	1:12:A:LEU:HD23	1:13:A:LYS:H	3	0.11	0.0	0.11
(3,25)	1:12:A:LEU:HD21	1:13:A:LYS:H	3	0.11	0.0	0.11
(3,25)	1:12:A:LEU:HD22	1:13:A:LYS:H	3	0.11	0.0	0.11
(3,25)	1:12:A:LEU:HD23	1:13:A:LYS:H	3	0.11	0.0	0.11
(3,169)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	3	0.11	0.0	0.11
(3,169)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	3	0.11	0.0	0.11
(3,169)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	3	0.11	0.0	0.11
(2,539)	1:21:A:ARG:HG2	1:22:A:PRO:HD2	2	1.51	0.0	1.51
(2,539)	1:21:A:ARG:HG3	1:22:A:PRO:HD2	2	1.51	0.0	1.51
(2,615)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	2	0.96	0.07	0.96
(2,615)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	2	0.96	0.07	0.96
(2,615)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	2	0.96	0.07	0.96
(2,615)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	2	0.96	0.07	0.96
(2,615)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	2	0.96	0.07	0.96
(2,615)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	2	0.96	0.07	0.96
(2,540)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	2	0.78	0.02	0.78
(2,540)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	2	0.78	0.02	0.78
(1,744)	1:7:A:LEU:HG	1:25:A:CYS:HB3	2	0.77	0.36	0.77
(3,668)	1:7:A:LEU:HG	1:25:A:CYS:HB3	2	0.77	0.36	0.77
(2,434)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.76	0.08	0.76
(2,189)	1:18:A:SER:H	1:19:A:SER:HB2	2	0.72	0.06	0.72
(2,580)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	2	0.66	0.01	0.66
(2,593)	1:5:A:VAL:HG11	1:6:A:ARG:H	2	0.6	0.01	0.6
(2,593)	1:5:A:VAL:HG12	1:6:A:ARG:H	2	0.6	0.01	0.6
(2,593)	1:5:A:VAL:HG13	1:6:A:ARG:H	2	0.6	0.01	0.6
(2,650)	1:8:A:TYR:HB2	1:25:A:CYS:HB2	2	0.52	0.08	0.52
(2,650)	1:8:A:TYR:HB3	1:25:A:CYS:HB2	2	0.52	0.08	0.52
(2,717)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	2	0.42	0.06	0.42
(2,106)	1:21:A:ARG:H	1:21:A:ARG:HB2	2	0.36	0.02	0.36
(2,49)	1:13:A:LYS:HA	1:13:A:LYS:HE2	2	0.28	0.07	0.28
(2,111)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	2	0.27	0.07	0.27
(1,448)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	2	0.22	0.1	0.22
(3,411)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	2	0.22	0.1	0.22
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD1	2	0.22	0.02	0.22
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD2	2	0.22	0.02	0.22
(2,549)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	2	0.22	0.02	0.22
(2,549)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	2	0.22	0.02	0.22
(2,549)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	2	0.22	0.02	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,549)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	2	0.22	0.02	0.22
(2,549)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	2	0.22	0.02	0.22
(2,549)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	2	0.22	0.02	0.22
(2,508)	1:14:A:ASP:HB3	1:19:A:SER:HA	2	0.19	0.08	0.19
(2,720)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	2	0.17	0.05	0.17
(2,59)	1:2:A:GLU:HB3	1:4:A:CYS:H	2	0.16	0.02	0.16
(2,137)	1:18:A:SER:HA	1:18:A:SER:HB3	2	0.16	0.06	0.16
(1,91)	1:4:A:CYS:HB2	1:5:A:VAL:H	2	0.15	0.01	0.15
(3,86)	1:4:A:CYS:HB2	1:5:A:VAL:H	2	0.15	0.01	0.15
(1,479)	1:15:A:GLY:HA3	1:16:A:GLY:H	2	0.15	0.0	0.15
(3,440)	1:15:A:GLY:HA3	1:16:A:GLY:H	2	0.15	0.0	0.15
(1,244)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.14	0.04	0.14
(2,273)	1:11:A:TRP:HE1	1:19:A:SER:HB3	2	0.14	0.02	0.14
(3,232)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.14	0.04	0.14
(1,601)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	2	0.14	0.02	0.14
(1,646)	1:10:A:GLN:HA	1:13:A:LYS:H	2	0.14	0.02	0.14
(3,545)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	2	0.14	0.02	0.14
(3,584)	1:10:A:GLN:HA	1:13:A:LYS:H	2	0.14	0.02	0.14
(1,15)	1:5:A:VAL:H	1:5:A:VAL:HG21	2	0.13	0.01	0.13
(1,15)	1:5:A:VAL:H	1:5:A:VAL:HG22	2	0.13	0.01	0.13
(1,15)	1:5:A:VAL:H	1:5:A:VAL:HG23	2	0.13	0.01	0.13
(1,31)	1:5:A:VAL:H	1:5:A:VAL:HG21	2	0.13	0.01	0.13
(1,31)	1:5:A:VAL:H	1:5:A:VAL:HG22	2	0.13	0.01	0.13
(1,31)	1:5:A:VAL:H	1:5:A:VAL:HG23	2	0.13	0.01	0.13
(2,250)	1:19:A:SER:HA	1:20:A:GLY:H	2	0.13	0.0	0.13
(3,14)	1:5:A:VAL:H	1:5:A:VAL:HG21	2	0.13	0.01	0.13
(3,14)	1:5:A:VAL:H	1:5:A:VAL:HG22	2	0.13	0.01	0.13
(3,14)	1:5:A:VAL:H	1:5:A:VAL:HG23	2	0.13	0.01	0.13
(3,29)	1:5:A:VAL:H	1:5:A:VAL:HG21	2	0.13	0.01	0.13
(3,29)	1:5:A:VAL:H	1:5:A:VAL:HG22	2	0.13	0.01	0.13
(3,29)	1:5:A:VAL:H	1:5:A:VAL:HG23	2	0.13	0.01	0.13
(1,187)	1:19:A:SER:H	1:19:A:SER:HG	2	0.12	0.01	0.12
(3,179)	1:19:A:SER:H	1:19:A:SER:HG	2	0.12	0.01	0.12
(1,222)	1:21:A:ARG:HA	1:22:A:PRO:HG2	2	0.12	0.01	0.12
(3,212)	1:21:A:ARG:HA	1:22:A:PRO:HG2	2	0.12	0.01	0.12
(1,35)	1:6:A:ARG:H	1:6:A:ARG:HG3	2	0.12	0.0	0.12
(3,33)	1:6:A:ARG:H	1:6:A:ARG:HG3	2	0.12	0.0	0.12
(1,553)	1:7:A:LEU:HA	1:10:A:GLN:HB3	2	0.11	0.0	0.11
(3,503)	1:7:A:LEU:HA	1:10:A:GLN:HB3	2	0.11	0.0	0.11
(1,449)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.11	0.0	0.11
(2,149)	1:10:A:GLN:HB3	1:10:A:GLN:HG2	2	0.11	0.0	0.11
(3,412)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.11	0.0	0.11

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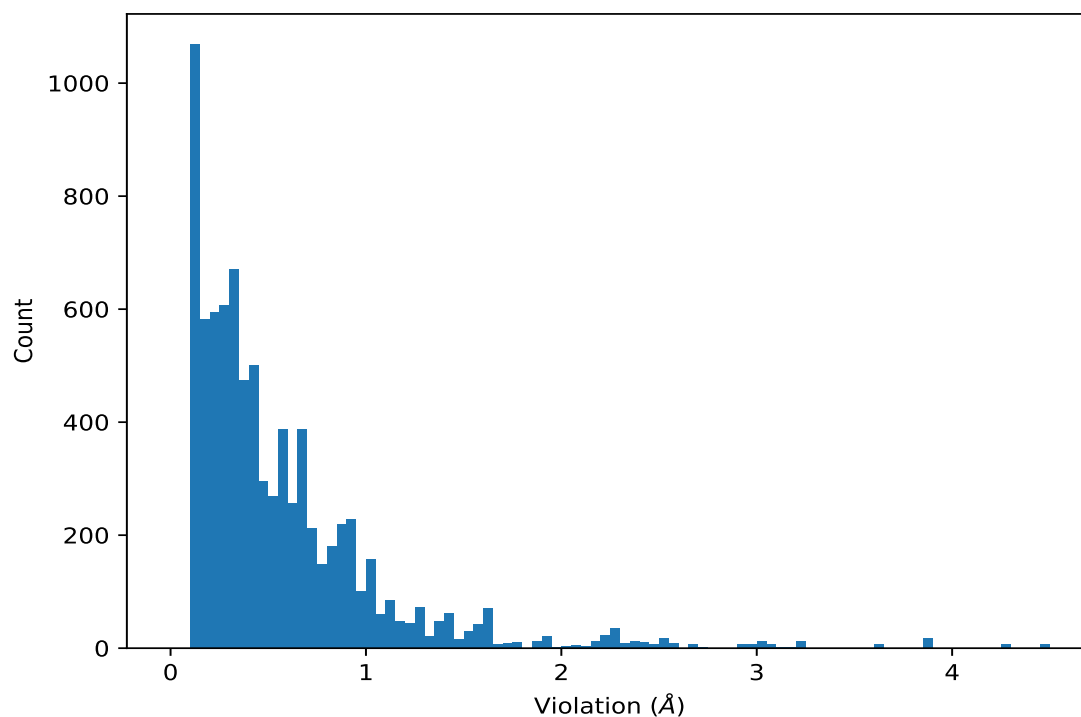
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,624)	1:8:A:TYR:HB2	1:12:A:LEU:H	2	0.1	0.0	0.1
(1,624)	1:8:A:TYR:HB3	1:12:A:LEU:H	2	0.1	0.0	0.1
(2,127)	1:9:A:ILE:HB	1:9:A:ILE:HG21	2	0.1	0.0	0.1
(2,127)	1:9:A:ILE:HB	1:9:A:ILE:HG22	2	0.1	0.0	0.1
(2,127)	1:9:A:ILE:HB	1:9:A:ILE:HG23	2	0.1	0.0	0.1
(3,565)	1:8:A:TYR:HB2	1:12:A:LEU:H	2	0.1	0.0	0.1
(3,565)	1:8:A:TYR:HB3	1:12:A:LEU:H	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)
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	1	4.46
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	1	4.46
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	1	4.46
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	1	4.46
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	1	4.46
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	1	4.46
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	8	4.28
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	8	4.28
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	8	4.28
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	8	4.28
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	8	4.28
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	8	4.28
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	3	3.9
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	3	3.9
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	3	3.9
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	3	3.9
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	3	3.9
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	3	3.9
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	8	3.9
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	8	3.9
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	8	3.9
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	8	3.9
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	8	3.9
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	8	3.9
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	1	3.89
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	1	3.89
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	1	3.89
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	1	3.89
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	1	3.89
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	1	3.89
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	3	3.61
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	3	3.61
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	3	3.61
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	3	3.61
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	3	3.61
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	3	3.61
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	2	3.22
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	2	3.22
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	2	3.22
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	2	3.22
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	2	3.22
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	2	3.22
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	4	3.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	4	3.2
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	4	3.2
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	4	3.2
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	4	3.2
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	4	3.2
(2,597)	1:21:A:ARG:HB3	1:21:A:ARG:HE	6	3.18
(2,597)	1:21:A:ARG:HB3	1:21:A:ARG:HE	5	3.14
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	6	3.08
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	6	3.08
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	6	3.08
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	6	3.08
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	6	3.08
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	6	3.08
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	9	3.05
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	9	3.05
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	9	3.05
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	9	3.05
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	9	3.05
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	9	3.05
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	7	3.03
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	7	3.03
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	7	3.03
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	7	3.03
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	7	3.03
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	7	3.03
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	5	2.97
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	5	2.97
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	5	2.97
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	5	2.97
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	5	2.97
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	5	2.97
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	10	2.92
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	10	2.92
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	10	2.92
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	10	2.92
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	10	2.92
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	10	2.92
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH21	10	2.72
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH22	10	2.72
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	2	2.68
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	2	2.68
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	2	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	2	2.68
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	2	2.68
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	2	2.68
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG2	5	2.58
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG3	5	2.58
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	10	2.57
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	10	2.57
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	10	2.57
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	10	2.57
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	10	2.57
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	10	2.57
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	5	2.53
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	5	2.53
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	5	2.53
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	5	2.53
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	5	2.53
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	5	2.53
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	7	2.51
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	7	2.51
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	7	2.51
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	7	2.51
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	7	2.51
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	7	2.51
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	9	2.5
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	9	2.5
(2,748)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	9	2.5
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG21	9	2.5
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG22	9	2.5
(2,748)	1:1:A:GLU:HG3	1:5:A:VAL:HG23	9	2.5
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	4	2.49
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	4	2.49
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	4	2.49
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	4	2.49
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	4	2.49
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	4	2.49
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG11	6	2.44
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG12	6	2.44
(2,749)	1:1:A:GLU:HG2	1:5:A:VAL:HG13	6	2.44
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG11	6	2.44
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG12	6	2.44
(2,749)	1:1:A:GLU:HG3	1:5:A:VAL:HG13	6	2.44
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG2	3	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG3	3	2.43
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG2	10	2.41
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG3	10	2.41
(3,609)	1:15:A:GLY:HA2	1:19:A:SER:HB3	4	2.4
(3,609)	1:15:A:GLY:HA2	1:19:A:SER:HB3	8	2.4
(3,609)	1:15:A:GLY:HA2	1:19:A:SER:HB3	10	2.4
(1,672)	1:15:A:GLY:HA2	1:19:A:SER:HB3	4	2.4
(1,672)	1:15:A:GLY:HA2	1:19:A:SER:HB3	8	2.4
(1,672)	1:15:A:GLY:HA2	1:19:A:SER:HB3	10	2.4
(3,609)	1:15:A:GLY:HA2	1:19:A:SER:HB3	9	2.38
(1,672)	1:15:A:GLY:HA2	1:19:A:SER:HB3	9	2.38
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG2	9	2.37
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG3	9	2.37
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG2	7	2.36
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG3	7	2.36
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG2	8	2.32
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG3	8	2.32
(4,71)	1:5:A:VAL:HG21	1:9:A:ILE:HB	7	2.31
(4,71)	1:5:A:VAL:HG22	1:9:A:ILE:HB	7	2.31
(4,71)	1:5:A:VAL:HG23	1:9:A:ILE:HB	7	2.31
(1,720)	1:5:A:VAL:HG21	1:9:A:ILE:HB	7	2.31
(1,720)	1:5:A:VAL:HG22	1:9:A:ILE:HB	7	2.31
(1,720)	1:5:A:VAL:HG23	1:9:A:ILE:HB	7	2.31
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH21	8	2.3
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH22	8	2.3
(4,71)	1:5:A:VAL:HG21	1:9:A:ILE:HB	8	2.29
(4,71)	1:5:A:VAL:HG22	1:9:A:ILE:HB	8	2.29
(4,71)	1:5:A:VAL:HG23	1:9:A:ILE:HB	8	2.29
(1,720)	1:5:A:VAL:HG21	1:9:A:ILE:HB	8	2.29
(1,720)	1:5:A:VAL:HG22	1:9:A:ILE:HB	8	2.29
(1,720)	1:5:A:VAL:HG23	1:9:A:ILE:HB	8	2.29
(4,60)	1:10:A:GLN:HA	1:11:A:TRP:HB2	3	2.27
(4,60)	1:10:A:GLN:HA	1:11:A:TRP:HB2	8	2.27
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG2	6	2.27
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG3	6	2.27
(1,636)	1:10:A:GLN:HA	1:11:A:TRP:HB2	3	2.27
(1,636)	1:10:A:GLN:HA	1:11:A:TRP:HB2	8	2.27
(4,60)	1:10:A:GLN:HA	1:11:A:TRP:HB2	1	2.26
(4,60)	1:10:A:GLN:HA	1:11:A:TRP:HB2	2	2.26
(4,60)	1:10:A:GLN:HA	1:11:A:TRP:HB2	4	2.26
(4,60)	1:10:A:GLN:HA	1:11:A:TRP:HB2	6	2.26
(4,60)	1:10:A:GLN:HA	1:11:A:TRP:HB2	7	2.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:10:A:GLN:HA	1:11:A:TRP:HB2	1	2.26
(1,636)	1:10:A:GLN:HA	1:11:A:TRP:HB2	2	2.26
(1,636)	1:10:A:GLN:HA	1:11:A:TRP:HB2	4	2.26
(1,636)	1:10:A:GLN:HA	1:11:A:TRP:HB2	6	2.26
(1,636)	1:10:A:GLN:HA	1:11:A:TRP:HB2	7	2.26
(4,71)	1:5:A:VAL:HG21	1:9:A:ILE:HB	5	2.25
(4,71)	1:5:A:VAL:HG22	1:9:A:ILE:HB	5	2.25
(4,71)	1:5:A:VAL:HG23	1:9:A:ILE:HB	5	2.25
(4,71)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	2.25
(4,71)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	2.25
(4,71)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	2.25
(1,720)	1:5:A:VAL:HG21	1:9:A:ILE:HB	5	2.25
(1,720)	1:5:A:VAL:HG22	1:9:A:ILE:HB	5	2.25
(1,720)	1:5:A:VAL:HG23	1:9:A:ILE:HB	5	2.25
(1,720)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	2.25
(1,720)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	2.25
(1,720)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	2.25
(4,71)	1:5:A:VAL:HG21	1:9:A:ILE:HB	9	2.24
(4,71)	1:5:A:VAL:HG22	1:9:A:ILE:HB	9	2.24
(4,71)	1:5:A:VAL:HG23	1:9:A:ILE:HB	9	2.24
(1,720)	1:5:A:VAL:HG21	1:9:A:ILE:HB	9	2.24
(1,720)	1:5:A:VAL:HG22	1:9:A:ILE:HB	9	2.24
(1,720)	1:5:A:VAL:HG23	1:9:A:ILE:HB	9	2.24
(4,71)	1:5:A:VAL:HG21	1:9:A:ILE:HB	2	2.23
(4,71)	1:5:A:VAL:HG22	1:9:A:ILE:HB	2	2.23
(4,71)	1:5:A:VAL:HG23	1:9:A:ILE:HB	2	2.23
(4,71)	1:5:A:VAL:HG21	1:9:A:ILE:HB	3	2.23
(4,71)	1:5:A:VAL:HG22	1:9:A:ILE:HB	3	2.23
(4,71)	1:5:A:VAL:HG23	1:9:A:ILE:HB	3	2.23
(1,720)	1:5:A:VAL:HG21	1:9:A:ILE:HB	2	2.23
(1,720)	1:5:A:VAL:HG22	1:9:A:ILE:HB	2	2.23
(1,720)	1:5:A:VAL:HG23	1:9:A:ILE:HB	2	2.23
(1,720)	1:5:A:VAL:HG21	1:9:A:ILE:HB	3	2.23
(1,720)	1:5:A:VAL:HG22	1:9:A:ILE:HB	3	2.23
(1,720)	1:5:A:VAL:HG23	1:9:A:ILE:HB	3	2.23
(4,60)	1:10:A:GLN:HA	1:11:A:TRP:HB2	5	2.22
(1,636)	1:10:A:GLN:HA	1:11:A:TRP:HB2	5	2.22
(4,60)	1:10:A:GLN:HA	1:11:A:TRP:HB2	9	2.2
(1,636)	1:10:A:GLN:HA	1:11:A:TRP:HB2	9	2.2
(4,71)	1:5:A:VAL:HG21	1:9:A:ILE:HB	1	2.19
(4,71)	1:5:A:VAL:HG22	1:9:A:ILE:HB	1	2.19
(4,71)	1:5:A:VAL:HG23	1:9:A:ILE:HB	1	2.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,60)	1:10:A:GLN:HA	1:11:A:TRP:HB2	10	2.19
(1,720)	1:5:A:VAL:HG21	1:9:A:ILE:HB	1	2.19
(1,720)	1:5:A:VAL:HG22	1:9:A:ILE:HB	1	2.19
(1,720)	1:5:A:VAL:HG23	1:9:A:ILE:HB	1	2.19
(1,636)	1:10:A:GLN:HA	1:11:A:TRP:HB2	10	2.19
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH21	8	2.18
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH22	8	2.18
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG2	2	2.18
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG3	2	2.18
(2,597)	1:21:A:ARG:HB3	1:21:A:ARG:HE	3	2.13
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG2	1	2.1
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG3	1	2.1
(4,64)	1:5:A:VAL:HA	1:25:A:CYS:HB3	6	2.06
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG2	4	2.06
(2,599)	1:21:A:ARG:HE	1:21:A:ARG:HG3	4	2.06
(2,597)	1:21:A:ARG:HB3	1:21:A:ARG:HE	7	2.06
(1,675)	1:5:A:VAL:HA	1:25:A:CYS:HB3	6	2.06
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH21	10	2.04
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH22	10	2.04
(2,597)	1:21:A:ARG:HB3	1:21:A:ARG:HE	2	2.04
(2,597)	1:21:A:ARG:HB3	1:21:A:ARG:HE	1	2.01
(2,597)	1:21:A:ARG:HB3	1:21:A:ARG:HE	10	1.96
(4,44)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	3	1.94
(4,44)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	4	1.94
(1,511)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	3	1.94
(1,511)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	4	1.94
(4,44)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	1	1.93
(4,44)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	2	1.93
(4,44)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	6	1.93
(4,44)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	8	1.93
(1,511)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	1	1.93
(1,511)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	2	1.93
(1,511)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	6	1.93
(1,511)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	8	1.93
(4,44)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	5	1.92
(4,44)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	7	1.92
(4,44)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	10	1.92
(1,511)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	5	1.92
(1,511)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	7	1.92
(1,511)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	10	1.92
(4,44)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	9	1.91
(2,597)	1:21:A:ARG:HB3	1:21:A:ARG:HE	9	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	9	1.91
(4,11)	1:9:A:ILE:HB	1:11:A:TRP:H	1	1.9
(2,597)	1:21:A:ARG:HB3	1:21:A:ARG:HE	4	1.9
(1,233)	1:9:A:ILE:HB	1:11:A:TRP:H	1	1.9
(4,11)	1:9:A:ILE:HB	1:11:A:TRP:H	2	1.89
(4,11)	1:9:A:ILE:HB	1:11:A:TRP:H	4	1.89
(1,233)	1:9:A:ILE:HB	1:11:A:TRP:H	2	1.89
(1,233)	1:9:A:ILE:HB	1:11:A:TRP:H	4	1.89
(4,11)	1:9:A:ILE:HB	1:11:A:TRP:H	3	1.86
(4,11)	1:9:A:ILE:HB	1:11:A:TRP:H	7	1.86
(2,597)	1:21:A:ARG:HB3	1:21:A:ARG:HE	8	1.86
(1,233)	1:9:A:ILE:HB	1:11:A:TRP:H	3	1.86
(1,233)	1:9:A:ILE:HB	1:11:A:TRP:H	7	1.86
(4,11)	1:9:A:ILE:HB	1:11:A:TRP:H	5	1.78
(4,11)	1:9:A:ILE:HB	1:11:A:TRP:H	8	1.78
(2,646)	1:15:A:GLY:HA2	1:19:A:SER:HB3	4	1.78
(2,646)	1:15:A:GLY:HA2	1:19:A:SER:HB3	8	1.78
(2,646)	1:15:A:GLY:HA2	1:19:A:SER:HB3	10	1.78
(1,233)	1:9:A:ILE:HB	1:11:A:TRP:H	5	1.78
(1,233)	1:9:A:ILE:HB	1:11:A:TRP:H	8	1.78
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH21	6	1.76
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH22	6	1.76
(2,646)	1:15:A:GLY:HA2	1:19:A:SER:HB3	9	1.75
(2,601)	1:24:A:PRO:HG2	1:25:A:CYS:H	2	1.74
(4,11)	1:9:A:ILE:HB	1:11:A:TRP:H	9	1.72
(2,601)	1:24:A:PRO:HG2	1:25:A:CYS:H	3	1.72
(2,601)	1:24:A:PRO:HG2	1:25:A:CYS:H	4	1.72
(2,601)	1:24:A:PRO:HG2	1:25:A:CYS:H	5	1.72
(1,233)	1:9:A:ILE:HB	1:11:A:TRP:H	9	1.72
(2,601)	1:24:A:PRO:HG2	1:25:A:CYS:H	7	1.71
(2,601)	1:24:A:PRO:HG2	1:25:A:CYS:H	8	1.71
(2,601)	1:24:A:PRO:HG2	1:25:A:CYS:H	9	1.71
(2,601)	1:24:A:PRO:HG2	1:25:A:CYS:H	10	1.7
(4,11)	1:9:A:ILE:HB	1:11:A:TRP:H	6	1.69
(2,601)	1:24:A:PRO:HG2	1:25:A:CYS:H	6	1.69
(1,233)	1:9:A:ILE:HB	1:11:A:TRP:H	6	1.69
(2,694)	1:5:A:VAL:HG21	1:9:A:ILE:HB	7	1.66
(2,694)	1:5:A:VAL:HG22	1:9:A:ILE:HB	7	1.66
(2,694)	1:5:A:VAL:HG23	1:9:A:ILE:HB	7	1.66
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	4	1.64
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	4	1.64
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	4	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	4	1.64
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	4	1.64
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	4	1.64
(4,39)	1:8:A:TYR:HD1	1:12:A:LEU:HG	3	1.64
(4,39)	1:8:A:TYR:HD2	1:12:A:LEU:HG	3	1.64
(2,694)	1:5:A:VAL:HG21	1:9:A:ILE:HB	8	1.64
(2,694)	1:5:A:VAL:HG22	1:9:A:ILE:HB	8	1.64
(2,694)	1:5:A:VAL:HG23	1:9:A:ILE:HB	8	1.64
(2,614)	1:10:A:GLN:HA	1:11:A:TRP:HB2	1	1.64
(2,614)	1:10:A:GLN:HA	1:11:A:TRP:HB2	3	1.64
(2,614)	1:10:A:GLN:HA	1:11:A:TRP:HB2	8	1.64
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	4	1.64
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	4	1.64
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	4	1.64
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	4	1.64
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	4	1.64
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	4	1.64
(1,451)	1:8:A:TYR:HD1	1:12:A:LEU:HG	3	1.64
(1,451)	1:8:A:TYR:HD2	1:12:A:LEU:HG	3	1.64
(4,71)	1:5:A:VAL:HG21	1:9:A:ILE:HB	6	1.63
(4,71)	1:5:A:VAL:HG22	1:9:A:ILE:HB	6	1.63
(4,71)	1:5:A:VAL:HG23	1:9:A:ILE:HB	6	1.63
(4,39)	1:8:A:TYR:HD1	1:12:A:LEU:HG	9	1.63
(4,39)	1:8:A:TYR:HD2	1:12:A:LEU:HG	9	1.63
(4,39)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	1.63
(4,39)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	1.63
(2,614)	1:10:A:GLN:HA	1:11:A:TRP:HB2	2	1.63
(2,614)	1:10:A:GLN:HA	1:11:A:TRP:HB2	4	1.63
(2,614)	1:10:A:GLN:HA	1:11:A:TRP:HB2	6	1.63
(2,614)	1:10:A:GLN:HA	1:11:A:TRP:HB2	7	1.63
(2,57)	1:3:A:GLU:HG2	1:4:A:CYS:H	1	1.63
(2,57)	1:3:A:GLU:HG3	1:4:A:CYS:H	1	1.63
(1,720)	1:5:A:VAL:HG21	1:9:A:ILE:HB	6	1.63
(1,720)	1:5:A:VAL:HG22	1:9:A:ILE:HB	6	1.63
(1,720)	1:5:A:VAL:HG23	1:9:A:ILE:HB	6	1.63
(1,451)	1:8:A:TYR:HD1	1:12:A:LEU:HG	9	1.63
(1,451)	1:8:A:TYR:HD2	1:12:A:LEU:HG	9	1.63
(1,451)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	1.63
(1,451)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	1.63
(4,71)	1:5:A:VAL:HG21	1:9:A:ILE:HB	4	1.62
(4,71)	1:5:A:VAL:HG22	1:9:A:ILE:HB	4	1.62
(4,71)	1:5:A:VAL:HG23	1:9:A:ILE:HB	4	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,39)	1:8:A:TYR:HD1	1:12:A:LEU:HG	6	1.62
(4,39)	1:8:A:TYR:HD2	1:12:A:LEU:HG	6	1.62
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH21	6	1.62
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH22	6	1.62
(1,720)	1:5:A:VAL:HG21	1:9:A:ILE:HB	4	1.62
(1,720)	1:5:A:VAL:HG22	1:9:A:ILE:HB	4	1.62
(1,720)	1:5:A:VAL:HG23	1:9:A:ILE:HB	4	1.62
(1,451)	1:8:A:TYR:HD1	1:12:A:LEU:HG	6	1.62
(1,451)	1:8:A:TYR:HD2	1:12:A:LEU:HG	6	1.62
(4,39)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	1.6
(4,39)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	1.6
(4,39)	1:8:A:TYR:HD1	1:12:A:LEU:HG	7	1.6
(4,39)	1:8:A:TYR:HD2	1:12:A:LEU:HG	7	1.6
(4,11)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.6
(2,694)	1:5:A:VAL:HG21	1:9:A:ILE:HB	5	1.6
(2,694)	1:5:A:VAL:HG22	1:9:A:ILE:HB	5	1.6
(2,694)	1:5:A:VAL:HG23	1:9:A:ILE:HB	5	1.6
(2,694)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	1.6
(2,694)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	1.6
(2,694)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	1.6
(1,451)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	1.6
(1,451)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	1.6
(1,451)	1:8:A:TYR:HD1	1:12:A:LEU:HG	7	1.6
(1,451)	1:8:A:TYR:HD2	1:12:A:LEU:HG	7	1.6
(1,233)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.6
(4,39)	1:8:A:TYR:HD1	1:12:A:LEU:HG	2	1.59
(4,39)	1:8:A:TYR:HD2	1:12:A:LEU:HG	2	1.59
(2,694)	1:5:A:VAL:HG21	1:9:A:ILE:HB	9	1.59
(2,694)	1:5:A:VAL:HG22	1:9:A:ILE:HB	9	1.59
(2,694)	1:5:A:VAL:HG23	1:9:A:ILE:HB	9	1.59
(2,614)	1:10:A:GLN:HA	1:11:A:TRP:HB2	5	1.59
(2,601)	1:24:A:PRO:HG2	1:25:A:CYS:H	1	1.59
(2,57)	1:3:A:GLU:HG2	1:4:A:CYS:H	6	1.59
(2,57)	1:3:A:GLU:HG3	1:4:A:CYS:H	6	1.59
(2,57)	1:3:A:GLU:HG2	1:4:A:CYS:H	7	1.59
(2,57)	1:3:A:GLU:HG3	1:4:A:CYS:H	7	1.59
(1,451)	1:8:A:TYR:HD1	1:12:A:LEU:HG	2	1.59
(1,451)	1:8:A:TYR:HD2	1:12:A:LEU:HG	2	1.59
(4,39)	1:8:A:TYR:HD1	1:12:A:LEU:HG	4	1.58
(4,39)	1:8:A:TYR:HD2	1:12:A:LEU:HG	4	1.58
(4,39)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	1.58
(4,39)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,694)	1:5:A:VAL:HG21	1:9:A:ILE:HB	2	1.58
(2,694)	1:5:A:VAL:HG22	1:9:A:ILE:HB	2	1.58
(2,694)	1:5:A:VAL:HG23	1:9:A:ILE:HB	2	1.58
(2,694)	1:5:A:VAL:HG21	1:9:A:ILE:HB	3	1.58
(2,694)	1:5:A:VAL:HG22	1:9:A:ILE:HB	3	1.58
(2,694)	1:5:A:VAL:HG23	1:9:A:ILE:HB	3	1.58
(1,451)	1:8:A:TYR:HD1	1:12:A:LEU:HG	4	1.58
(1,451)	1:8:A:TYR:HD2	1:12:A:LEU:HG	4	1.58
(1,451)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	1.58
(1,451)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	1.58
(4,39)	1:8:A:TYR:HD1	1:12:A:LEU:HG	1	1.57
(4,39)	1:8:A:TYR:HD2	1:12:A:LEU:HG	1	1.57
(2,614)	1:10:A:GLN:HA	1:11:A:TRP:HB2	9	1.57
(2,614)	1:10:A:GLN:HA	1:11:A:TRP:HB2	10	1.57
(2,466)	1:17:A:PRO:HA	1:18:A:SER:H	7	1.57
(2,57)	1:3:A:GLU:HG2	1:4:A:CYS:H	4	1.57
(2,57)	1:3:A:GLU:HG3	1:4:A:CYS:H	4	1.57
(1,451)	1:8:A:TYR:HD1	1:12:A:LEU:HG	1	1.57
(1,451)	1:8:A:TYR:HD2	1:12:A:LEU:HG	1	1.57
(2,57)	1:3:A:GLU:HG2	1:4:A:CYS:H	10	1.56
(2,57)	1:3:A:GLU:HG3	1:4:A:CYS:H	10	1.56
(4,49)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	5	1.55
(2,57)	1:3:A:GLU:HG2	1:4:A:CYS:H	8	1.55
(2,57)	1:3:A:GLU:HG3	1:4:A:CYS:H	8	1.55
(1,534)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	5	1.55
(4,49)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	2	1.54
(2,694)	1:5:A:VAL:HG21	1:9:A:ILE:HB	1	1.54
(2,694)	1:5:A:VAL:HG22	1:9:A:ILE:HB	1	1.54
(2,694)	1:5:A:VAL:HG23	1:9:A:ILE:HB	1	1.54
(1,534)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	2	1.54
(4,49)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	3	1.52
(1,534)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	3	1.52
(2,539)	1:21:A:ARG:HG2	1:22:A:PRO:HD2	8	1.51
(2,539)	1:21:A:ARG:HG3	1:22:A:PRO:HD2	8	1.51
(2,539)	1:21:A:ARG:HG2	1:22:A:PRO:HD2	10	1.51
(2,539)	1:21:A:ARG:HG3	1:22:A:PRO:HD2	10	1.51
(2,526)	1:4:A:CYS:HA	1:7:A:LEU:HG	2	1.51
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	6	1.5
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	6	1.5
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	6	1.5
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	6	1.5
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	6	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	6	1.5
(4,49)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	6	1.5
(2,526)	1:4:A:CYS:HA	1:7:A:LEU:HG	5	1.5
(2,57)	1:3:A:GLU:HG2	1:4:A:CYS:H	3	1.5
(2,57)	1:3:A:GLU:HG3	1:4:A:CYS:H	3	1.5
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	6	1.5
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	6	1.5
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	6	1.5
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	6	1.5
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	6	1.5
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	6	1.5
(1,534)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	6	1.5
(2,526)	1:4:A:CYS:HA	1:7:A:LEU:HG	3	1.49
(2,526)	1:4:A:CYS:HA	1:7:A:LEU:HG	9	1.49
(2,223)	1:3:A:GLU:H	1:4:A:CYS:H	9	1.49
(2,57)	1:3:A:GLU:HG2	1:4:A:CYS:H	5	1.49
(2,57)	1:3:A:GLU:HG3	1:4:A:CYS:H	5	1.49
(4,49)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	10	1.47
(3,609)	1:15:A:GLY:HA2	1:19:A:SER:HB3	2	1.47
(2,526)	1:4:A:CYS:HA	1:7:A:LEU:HG	10	1.47
(2,223)	1:3:A:GLU:H	1:4:A:CYS:H	2	1.47
(1,672)	1:15:A:GLY:HA2	1:19:A:SER:HB3	2	1.47
(1,534)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	10	1.47
(4,49)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	9	1.46
(2,574)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	6	1.46
(2,504)	1:14:A:ASP:HB3	1:19:A:SER:HB2	10	1.46
(1,534)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	9	1.46
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	10	1.45
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	10	1.45
(4,49)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	1	1.44
(4,49)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	8	1.44
(3,616)	1:17:A:PRO:HB2	1:18:A:SER:HB3	5	1.44
(1,682)	1:17:A:PRO:HB2	1:18:A:SER:HB3	5	1.44
(1,534)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	1	1.44
(1,534)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	8	1.44
(4,23)	1:22:A:PRO:HA	1:23:A:PRO:HG2	7	1.43
(2,649)	1:5:A:VAL:HA	1:25:A:CYS:HB3	6	1.43
(2,505)	1:4:A:CYS:HB2	1:25:A:CYS:HB2	7	1.43
(1,348)	1:22:A:PRO:HA	1:23:A:PRO:HG2	7	1.43
(4,49)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	7	1.42
(4,23)	1:22:A:PRO:HA	1:23:A:PRO:HG2	8	1.42
(4,23)	1:22:A:PRO:HA	1:23:A:PRO:HG2	10	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,609)	1:15:A:GLY:HA2	1:19:A:SER:HB3	7	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD11	1	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD12	1	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD13	1	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD11	2	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD12	2	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD13	2	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD11	3	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD12	3	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD13	3	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD11	4	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD12	4	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD13	4	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD11	6	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD12	6	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD13	6	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD11	8	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD12	8	1.42
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD13	8	1.42
(2,575)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	9	1.42
(1,672)	1:15:A:GLY:HA2	1:19:A:SER:HB3	7	1.42
(1,534)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	7	1.42
(1,348)	1:22:A:PRO:HA	1:23:A:PRO:HG2	8	1.42
(1,348)	1:22:A:PRO:HA	1:23:A:PRO:HG2	10	1.42
(4,23)	1:22:A:PRO:HA	1:23:A:PRO:HG2	9	1.41
(3,609)	1:15:A:GLY:HA2	1:19:A:SER:HB3	1	1.41
(3,609)	1:15:A:GLY:HA2	1:19:A:SER:HB3	3	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD11	5	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD12	5	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD13	5	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD11	7	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD12	7	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD13	7	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD11	9	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD12	9	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD13	9	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD11	10	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD12	10	1.41
(2,664)	1:9:A:ILE:HA	1:12:A:LEU:HD13	10	1.41
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	3	1.41
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	3	1.41
(2,505)	1:4:A:CYS:HB2	1:25:A:CYS:HB2	8	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,57)	1:3:A:GLU:HG2	1:4:A:CYS:H	9	1.41
(2,57)	1:3:A:GLU:HG3	1:4:A:CYS:H	9	1.41
(1,672)	1:15:A:GLY:HA2	1:19:A:SER:HB3	1	1.41
(1,672)	1:15:A:GLY:HA2	1:19:A:SER:HB3	3	1.41
(1,348)	1:22:A:PRO:HA	1:23:A:PRO:HG2	9	1.41
(4,23)	1:22:A:PRO:HA	1:23:A:PRO:HG2	1	1.4
(1,348)	1:22:A:PRO:HA	1:23:A:PRO:HG2	1	1.4
(3,609)	1:15:A:GLY:HA2	1:19:A:SER:HB3	5	1.39
(3,90)	1:2:A:GLU:HG2	1:6:A:ARG:H	7	1.39
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	6	1.39
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	6	1.39
(2,57)	1:3:A:GLU:HG2	1:4:A:CYS:H	2	1.39
(2,57)	1:3:A:GLU:HG3	1:4:A:CYS:H	2	1.39
(1,672)	1:15:A:GLY:HA2	1:19:A:SER:HB3	5	1.39
(1,95)	1:2:A:GLU:HG2	1:6:A:ARG:H	7	1.39
(4,23)	1:22:A:PRO:HA	1:23:A:PRO:HG2	5	1.38
(3,616)	1:17:A:PRO:HB2	1:18:A:SER:HB3	7	1.38
(2,526)	1:4:A:CYS:HA	1:7:A:LEU:HG	8	1.38
(1,682)	1:17:A:PRO:HB2	1:18:A:SER:HB3	7	1.38
(1,348)	1:22:A:PRO:HA	1:23:A:PRO:HG2	5	1.38
(4,49)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	4	1.37
(4,23)	1:22:A:PRO:HA	1:23:A:PRO:HG2	3	1.37
(3,616)	1:17:A:PRO:HB2	1:18:A:SER:HB3	1	1.37
(3,616)	1:17:A:PRO:HB2	1:18:A:SER:HB3	2	1.37
(3,90)	1:2:A:GLU:HG2	1:6:A:ARG:H	6	1.37
(1,682)	1:17:A:PRO:HB2	1:18:A:SER:HB3	1	1.37
(1,682)	1:17:A:PRO:HB2	1:18:A:SER:HB3	2	1.37
(1,534)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	4	1.37
(1,348)	1:22:A:PRO:HA	1:23:A:PRO:HG2	3	1.37
(1,95)	1:2:A:GLU:HG2	1:6:A:ARG:H	6	1.37
(4,47)	1:12:A:LEU:HD21	1:13:A:LYS:HA	5	1.36
(4,47)	1:12:A:LEU:HD22	1:13:A:LYS:HA	5	1.36
(4,47)	1:12:A:LEU:HD23	1:13:A:LYS:HA	5	1.36
(3,609)	1:15:A:GLY:HA2	1:19:A:SER:HB3	6	1.36
(2,526)	1:4:A:CYS:HA	1:7:A:LEU:HG	7	1.36
(1,672)	1:15:A:GLY:HA2	1:19:A:SER:HB3	6	1.36
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:HA	5	1.36
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:HA	5	1.36
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:HA	5	1.36
(4,23)	1:22:A:PRO:HA	1:23:A:PRO:HG2	2	1.35
(4,23)	1:22:A:PRO:HA	1:23:A:PRO:HG2	6	1.35
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	4	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	4	1.35
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	4	1.35
(3,90)	1:2:A:GLU:HG2	1:6:A:ARG:H	1	1.35
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	5	1.35
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	5	1.35
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	4	1.35
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	4	1.35
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	4	1.35
(1,348)	1:22:A:PRO:HA	1:23:A:PRO:HG2	2	1.35
(1,348)	1:22:A:PRO:HA	1:23:A:PRO:HG2	6	1.35
(1,95)	1:2:A:GLU:HG2	1:6:A:ARG:H	1	1.35
(4,48)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	10	1.33
(1,533)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	10	1.33
(4,48)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	6	1.32
(2,575)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	7	1.32
(2,223)	1:3:A:GLU:H	1:4:A:CYS:H	3	1.32
(1,533)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	6	1.32
(4,64)	1:5:A:VAL:HA	1:25:A:CYS:HB3	4	1.31
(3,184)	1:18:A:SER:H	1:19:A:SER:HB2	7	1.31
(1,675)	1:5:A:VAL:HA	1:25:A:CYS:HB3	4	1.31
(1,193)	1:18:A:SER:H	1:19:A:SER:HB2	7	1.31
(4,47)	1:12:A:LEU:HD21	1:13:A:LYS:HA	7	1.3
(4,47)	1:12:A:LEU:HD22	1:13:A:LYS:HA	7	1.3
(4,47)	1:12:A:LEU:HD23	1:13:A:LYS:HA	7	1.3
(3,671)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	3	1.3
(3,671)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	9	1.3
(2,223)	1:3:A:GLU:H	1:4:A:CYS:H	4	1.3
(1,750)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	3	1.3
(1,750)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	9	1.3
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:HA	7	1.3
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:HA	7	1.3
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:HA	7	1.3
(4,48)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	1	1.29
(4,48)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	3	1.29
(3,671)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	2	1.29
(3,671)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	5	1.29
(3,369)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	1.29
(3,90)	1:2:A:GLU:HG2	1:6:A:ARG:H	9	1.29
(1,750)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	2	1.29
(1,750)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	5	1.29
(1,533)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	1	1.29
(1,533)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	3	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	1.29
(1,95)	1:2:A:GLU:HG2	1:6:A:ARG:H	9	1.29
(4,48)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	5	1.28
(4,47)	1:12:A:LEU:HD21	1:13:A:LYS:HA	8	1.28
(4,47)	1:12:A:LEU:HD22	1:13:A:LYS:HA	8	1.28
(4,47)	1:12:A:LEU:HD23	1:13:A:LYS:HA	8	1.28
(4,47)	1:12:A:LEU:HD21	1:13:A:LYS:HA	9	1.28
(4,47)	1:12:A:LEU:HD22	1:13:A:LYS:HA	9	1.28
(4,47)	1:12:A:LEU:HD23	1:13:A:LYS:HA	9	1.28
(3,671)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	4	1.28
(3,669)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	6	1.28
(3,669)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	6	1.28
(2,223)	1:3:A:GLU:H	1:4:A:CYS:H	5	1.28
(1,750)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	4	1.28
(1,745)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	6	1.28
(1,745)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	6	1.28
(1,533)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	5	1.28
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:HA	8	1.28
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:HA	8	1.28
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:HA	8	1.28
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:HA	9	1.28
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:HA	9	1.28
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:HA	9	1.28
(4,48)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	8	1.27
(4,47)	1:12:A:LEU:HD21	1:13:A:LYS:HA	3	1.27
(4,47)	1:12:A:LEU:HD22	1:13:A:LYS:HA	3	1.27
(4,47)	1:12:A:LEU:HD23	1:13:A:LYS:HA	3	1.27
(3,671)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	10	1.27
(3,369)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	1.27
(1,750)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	10	1.27
(1,533)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	8	1.27
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:HA	3	1.27
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:HA	3	1.27
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:HA	3	1.27
(1,393)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	1.27
(4,48)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	2	1.26
(4,48)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	9	1.26
(4,47)	1:12:A:LEU:HD21	1:13:A:LYS:HA	4	1.26
(4,47)	1:12:A:LEU:HD22	1:13:A:LYS:HA	4	1.26
(4,47)	1:12:A:LEU:HD23	1:13:A:LYS:HA	4	1.26
(3,369)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	1.26
(3,369)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,526)	1:4:A:CYS:HA	1:7:A:LEU:HG	1	1.26
(2,526)	1:4:A:CYS:HA	1:7:A:LEU:HG	4	1.26
(2,227)	1:9:A:ILE:HB	1:11:A:TRP:H	1	1.26
(2,223)	1:3:A:GLU:H	1:4:A:CYS:H	10	1.26
(1,533)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	2	1.26
(1,533)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	9	1.26
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:HA	4	1.26
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:HA	4	1.26
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:HA	4	1.26
(1,393)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	1.26
(1,393)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.26
(3,369)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	1.25
(3,369)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	1.25
(3,369)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	1.25
(3,369)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	1.25
(2,573)	1:21:A:ARG:HD3	1:21:A:ARG:HE	4	1.25
(1,393)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	1.25
(1,393)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	1.25
(1,393)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	1.25
(1,393)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	1.25
(3,616)	1:17:A:PRO:HB2	1:18:A:SER:HB3	10	1.24
(3,369)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	1.24
(3,369)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	1.24
(2,573)	1:21:A:ARG:HD3	1:21:A:ARG:HE	1	1.24
(2,526)	1:4:A:CYS:HA	1:7:A:LEU:HG	6	1.24
(2,423)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	1	1.24
(2,423)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	1	1.24
(2,252)	1:10:A:GLN:HA	1:10:A:GLN:HE21	9	1.24
(2,227)	1:9:A:ILE:HB	1:11:A:TRP:H	2	1.24
(2,227)	1:9:A:ILE:HB	1:11:A:TRP:H	4	1.24
(2,223)	1:3:A:GLU:H	1:4:A:CYS:H	6	1.24
(1,682)	1:17:A:PRO:HB2	1:18:A:SER:HB3	10	1.24
(1,393)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	1.24
(1,393)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	1.24
(4,48)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	7	1.23
(4,47)	1:12:A:LEU:HD21	1:13:A:LYS:HA	10	1.23
(4,47)	1:12:A:LEU:HD22	1:13:A:LYS:HA	10	1.23
(4,47)	1:12:A:LEU:HD23	1:13:A:LYS:HA	10	1.23
(1,533)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	7	1.23
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:HA	10	1.23
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:HA	10	1.23
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:HA	10	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,47)	1:12:A:LEU:HD21	1:13:A:LYS:HA	6	1.22
(4,47)	1:12:A:LEU:HD22	1:13:A:LYS:HA	6	1.22
(4,47)	1:12:A:LEU:HD23	1:13:A:LYS:HA	6	1.22
(2,628)	1:14:A:ASP:HB3	1:15:A:GLY:H	10	1.22
(2,223)	1:3:A:GLU:H	1:4:A:CYS:H	7	1.22
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:HA	6	1.22
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:HA	6	1.22
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:HA	6	1.22
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	2	1.21
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	2	1.21
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	2	1.21
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	4	1.21
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	4	1.21
(2,505)	1:4:A:CYS:HB2	1:25:A:CYS:HB2	1	1.21
(2,477)	1:18:A:SER:H	1:19:A:SER:H	1	1.21
(2,477)	1:18:A:SER:H	1:19:A:SER:H	2	1.21
(2,477)	1:18:A:SER:H	1:19:A:SER:H	5	1.21
(2,227)	1:9:A:ILE:HB	1:11:A:TRP:H	3	1.21
(2,227)	1:9:A:ILE:HB	1:11:A:TRP:H	7	1.21
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	2	1.21
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	2	1.21
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	2	1.21
(4,47)	1:12:A:LEU:HD21	1:13:A:LYS:HA	1	1.2
(4,47)	1:12:A:LEU:HD22	1:13:A:LYS:HA	1	1.2
(4,47)	1:12:A:LEU:HD23	1:13:A:LYS:HA	1	1.2
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	5	1.2
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	5	1.2
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	5	1.2
(2,459)	1:14:A:ASP:HB2	1:15:A:GLY:H	5	1.2
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	5	1.2
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	5	1.2
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	5	1.2
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:HA	1	1.2
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:HA	1	1.2
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:HA	1	1.2
(4,78)	1:5:A:VAL:HB	1:9:A:ILE:HG12	8	1.19
(4,78)	1:5:A:VAL:HB	1:9:A:ILE:HG12	9	1.19
(3,616)	1:17:A:PRO:HB2	1:18:A:SER:HB3	8	1.19
(3,572)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	1.19
(3,184)	1:18:A:SER:H	1:19:A:SER:HB2	6	1.19
(2,573)	1:21:A:ARG:HD3	1:21:A:ARG:HE	2	1.19
(1,748)	1:5:A:VAL:HB	1:9:A:ILE:HG12	8	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,748)	1:5:A:VAL:HB	1:9:A:ILE:HG12	9	1.19
(1,682)	1:17:A:PRO:HB2	1:18:A:SER:HB3	8	1.19
(1,631)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	1.19
(1,193)	1:18:A:SER:H	1:19:A:SER:HB2	6	1.19
(4,78)	1:5:A:VAL:HB	1:9:A:ILE:HG12	3	1.18
(4,78)	1:5:A:VAL:HB	1:9:A:ILE:HG12	4	1.18
(4,78)	1:5:A:VAL:HB	1:9:A:ILE:HG12	5	1.18
(2,459)	1:14:A:ASP:HB2	1:15:A:GLY:H	8	1.18
(2,423)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	7	1.18
(2,423)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	7	1.18
(2,252)	1:10:A:GLN:HA	1:10:A:GLN:HE21	6	1.18
(1,748)	1:5:A:VAL:HB	1:9:A:ILE:HG12	3	1.18
(1,748)	1:5:A:VAL:HB	1:9:A:ILE:HG12	4	1.18
(1,748)	1:5:A:VAL:HB	1:9:A:ILE:HG12	5	1.18
(4,78)	1:5:A:VAL:HB	1:9:A:ILE:HG12	10	1.17
(2,423)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	6	1.17
(2,423)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	6	1.17
(1,748)	1:5:A:VAL:HB	1:9:A:ILE:HG12	10	1.17
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	3	1.16
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	3	1.16
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	3	1.16
(2,252)	1:10:A:GLN:HA	1:10:A:GLN:HE21	8	1.16
(2,242)	1:17:A:PRO:HB2	1:18:A:SER:H	9	1.16
(2,223)	1:3:A:GLU:H	1:4:A:CYS:H	8	1.16
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	3	1.16
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	3	1.16
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	3	1.16
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	9	1.15
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	9	1.15
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	9	1.15
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	9	1.15
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	9	1.15
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	9	1.15
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	9	1.15
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	9	1.15
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	9	1.15
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	8	1.15
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	8	1.15
(2,477)	1:18:A:SER:H	1:19:A:SER:H	3	1.15
(2,459)	1:14:A:ASP:HB2	1:15:A:GLY:H	4	1.15
(2,423)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	4	1.15
(2,423)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	4	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,423)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	8	1.15
(2,423)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	8	1.15
(2,252)	1:10:A:GLN:HA	1:10:A:GLN:HE21	10	1.15
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	9	1.15
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	9	1.15
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	9	1.15
(4,78)	1:5:A:VAL:HB	1:9:A:ILE:HG12	7	1.14
(4,47)	1:12:A:LEU:HD21	1:13:A:LYS:HA	2	1.14
(4,47)	1:12:A:LEU:HD22	1:13:A:LYS:HA	2	1.14
(4,47)	1:12:A:LEU:HD23	1:13:A:LYS:HA	2	1.14
(2,423)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	3	1.14
(2,423)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	3	1.14
(2,252)	1:10:A:GLN:HA	1:10:A:GLN:HE21	4	1.14
(1,748)	1:5:A:VAL:HB	1:9:A:ILE:HG12	7	1.14
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:HA	2	1.14
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:HA	2	1.14
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:HA	2	1.14
(3,668)	1:7:A:LEU:HG	1:25:A:CYS:HB3	1	1.13
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	10	1.13
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	10	1.13
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	10	1.13
(2,459)	1:14:A:ASP:HB2	1:15:A:GLY:H	2	1.13
(2,227)	1:9:A:ILE:HB	1:11:A:TRP:H	5	1.13
(2,227)	1:9:A:ILE:HB	1:11:A:TRP:H	8	1.13
(1,744)	1:7:A:LEU:HG	1:25:A:CYS:HB3	1	1.13
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	10	1.13
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	10	1.13
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	10	1.13
(4,78)	1:5:A:VAL:HB	1:9:A:ILE:HG12	6	1.12
(2,459)	1:14:A:ASP:HB2	1:15:A:GLY:H	3	1.12
(2,459)	1:14:A:ASP:HB2	1:15:A:GLY:H	9	1.12
(2,404)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	8	1.12
(2,404)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	8	1.12
(1,748)	1:5:A:VAL:HB	1:9:A:ILE:HG12	6	1.12
(4,13)	1:7:A:LEU:HG	1:25:A:CYS:H	10	1.11
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	9	1.11
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	9	1.11
(2,574)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	5	1.11
(2,459)	1:14:A:ASP:HB2	1:15:A:GLY:H	6	1.11
(2,423)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	9	1.11
(2,423)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	9	1.11
(1,252)	1:7:A:LEU:HG	1:25:A:CYS:H	10	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,78)	1:5:A:VAL:HB	1:9:A:ILE:HG12	2	1.1
(4,43)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	1	1.1
(4,43)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	2	1.1
(4,43)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	3	1.1
(4,43)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	4	1.1
(4,43)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	5	1.1
(4,43)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	6	1.1
(4,43)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	7	1.1
(4,43)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	8	1.1
(4,43)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	9	1.1
(4,43)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	10	1.1
(2,459)	1:14:A:ASP:HB2	1:15:A:GLY:H	1	1.1
(2,423)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	10	1.1
(2,423)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	10	1.1
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG2	5	1.1
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG3	5	1.1
(1,748)	1:5:A:VAL:HB	1:9:A:ILE:HG12	2	1.1
(1,510)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	1	1.1
(1,510)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	2	1.1
(1,510)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	3	1.1
(1,510)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	4	1.1
(1,510)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	5	1.1
(1,510)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	6	1.1
(1,510)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	7	1.1
(1,510)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	8	1.1
(1,510)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	9	1.1
(1,510)	1:11:A:TRP:HZ2	1:11:A:TRP:HZ3	10	1.1
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	8	1.09
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	8	1.09
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	8	1.09
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	8	1.09
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	8	1.09
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	8	1.09
(2,243)	1:17:A:PRO:HG2	1:18:A:SER:H	6	1.09
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	8	1.09
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	8	1.09
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	8	1.09
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	8	1.09
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	8	1.09
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	8	1.09
(3,90)	1:2:A:GLU:HG2	1:6:A:ARG:H	8	1.08
(3,90)	1:2:A:GLU:HG2	1:6:A:ARG:H	10	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,252)	1:10:A:GLN:HA	1:10:A:GLN:HE21	5	1.08
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG2	6	1.08
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG3	6	1.08
(1,95)	1:2:A:GLU:HG2	1:6:A:ARG:H	8	1.08
(1,95)	1:2:A:GLU:HG2	1:6:A:ARG:H	10	1.08
(4,76)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	6	1.07
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	4	1.07
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	4	1.07
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	4	1.07
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	4	1.07
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	4	1.07
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	4	1.07
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	4	1.07
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	4	1.07
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	4	1.07
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	4	1.07
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	4	1.07
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	4	1.07
(2,423)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	5	1.07
(2,423)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	5	1.07
(2,227)	1:9:A:ILE:HB	1:11:A:TRP:H	9	1.07
(2,184)	1:19:A:SER:HG	1:21:A:ARG:H	8	1.07
(1,743)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	6	1.07
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	4	1.07
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	4	1.07
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	4	1.07
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	4	1.07
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	4	1.07
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	4	1.07
(4,16)	1:11:A:TRP:H	1:12:A:LEU:HA	2	1.06
(3,90)	1:2:A:GLU:HG2	1:6:A:ARG:H	3	1.06
(2,741)	1:2:A:GLU:HA	1:5:A:VAL:H	3	1.06
(2,423)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	2	1.06
(2,423)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	2	1.06
(2,252)	1:10:A:GLN:HA	1:10:A:GLN:HE21	2	1.06
(1,274)	1:11:A:TRP:H	1:12:A:LEU:HA	2	1.06
(1,95)	1:2:A:GLU:HG2	1:6:A:ARG:H	3	1.06
(4,68)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	7	1.05
(4,68)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	7	1.05
(4,68)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	7	1.05
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG2	4	1.05
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG3	4	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,711)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	7	1.05
(1,711)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	7	1.05
(1,711)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	7	1.05
(4,68)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	8	1.04
(4,68)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	8	1.04
(4,68)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	8	1.04
(4,23)	1:22:A:PRO:HA	1:23:A:PRO:HG2	4	1.04
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	10	1.04
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	10	1.04
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	10	1.04
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	10	1.04
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	10	1.04
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	10	1.04
(2,574)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	8	1.04
(2,404)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	1	1.04
(2,404)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	1	1.04
(2,392)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	1	1.04
(2,392)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	1	1.04
(2,227)	1:9:A:ILE:HB	1:11:A:TRP:H	6	1.04
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD11	2	1.04
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD12	2	1.04
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD13	2	1.04
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD11	3	1.04
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD12	3	1.04
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD13	3	1.04
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD11	6	1.04
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD12	6	1.04
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD13	6	1.04
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	2	1.04
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	2	1.04
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	2	1.04
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	3	1.04
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	3	1.04
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	3	1.04
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	6	1.04
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	6	1.04
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	6	1.04
(1,711)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	8	1.04
(1,711)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	8	1.04
(1,711)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	8	1.04
(1,348)	1:22:A:PRO:HA	1:23:A:PRO:HG2	4	1.04
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	7	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	7	1.03
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	7	1.03
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	7	1.03
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	7	1.03
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	7	1.03
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	9	1.03
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	9	1.03
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	9	1.03
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	9	1.03
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	9	1.03
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	9	1.03
(4,16)	1:11:A:TRP:H	1:12:A:LEU:HA	1	1.03
(3,616)	1:17:A:PRO:HB2	1:18:A:SER:HB3	9	1.03
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	6	1.03
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	6	1.03
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	6	1.03
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	6	1.03
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	6	1.03
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	6	1.03
(2,615)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	4	1.03
(2,615)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	4	1.03
(2,615)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	4	1.03
(2,615)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	4	1.03
(2,615)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	4	1.03
(2,615)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	4	1.03
(2,575)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	1	1.03
(2,575)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	2	1.03
(2,537)	1:8:A:TYR:HA	1:24:A:PRO:HG2	2	1.03
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG2	8	1.03
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG3	8	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD11	4	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD12	4	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD13	4	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD11	5	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD12	5	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD13	5	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD11	10	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD12	10	1.03
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD13	10	1.03
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	4	1.03
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	4	1.03
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	4	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	5	1.03
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	5	1.03
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	5	1.03
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	10	1.03
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	10	1.03
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	10	1.03
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	7	1.03
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	7	1.03
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	7	1.03
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	7	1.03
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	7	1.03
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	7	1.03
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	9	1.03
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	9	1.03
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	9	1.03
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	9	1.03
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	9	1.03
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	9	1.03
(1,682)	1:17:A:PRO:HB2	1:18:A:SER:HB3	9	1.03
(1,274)	1:11:A:TRP:H	1:12:A:LEU:HA	1	1.03
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	1	1.02
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	1	1.02
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	1	1.02
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	1	1.02
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	1	1.02
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	1	1.02
(4,64)	1:5:A:VAL:HA	1:25:A:CYS:HB3	1	1.02
(4,16)	1:11:A:TRP:H	1:12:A:LEU:HA	4	1.02
(2,710)	1:9:A:ILE:HA	1:12:A:LEU:HB2	10	1.02
(2,537)	1:8:A:TYR:HA	1:24:A:PRO:HG2	3	1.02
(2,537)	1:8:A:TYR:HA	1:24:A:PRO:HG2	5	1.02
(2,537)	1:8:A:TYR:HA	1:24:A:PRO:HG2	9	1.02
(2,537)	1:8:A:TYR:HA	1:24:A:PRO:HG2	10	1.02
(2,357)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	4	1.02
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG2	1	1.02
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG3	1	1.02
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG2	3	1.02
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG3	3	1.02
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG2	9	1.02
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG3	9	1.02
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG2	1	1.02
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG3	1	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	1	1.02
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	1	1.02
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	1	1.02
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	1	1.02
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	1	1.02
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	1	1.02
(1,675)	1:5:A:VAL:HA	1:25:A:CYS:HB3	1	1.02
(1,274)	1:11:A:TRP:H	1:12:A:LEU:HA	4	1.02
(4,50)	1:4:A:CYS:HA	1:7:A:LEU:HB3	1	1.01
(4,16)	1:11:A:TRP:H	1:12:A:LEU:HA	3	1.01
(3,669)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	4	1.01
(3,669)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	4	1.01
(3,90)	1:2:A:GLU:HG2	1:6:A:ARG:H	5	1.01
(2,710)	1:9:A:ILE:HA	1:12:A:LEU:HB2	2	1.01
(2,710)	1:9:A:ILE:HA	1:12:A:LEU:HB2	6	1.01
(2,710)	1:9:A:ILE:HA	1:12:A:LEU:HB2	9	1.01
(2,537)	1:8:A:TYR:HA	1:24:A:PRO:HG2	4	1.01
(2,537)	1:8:A:TYR:HA	1:24:A:PRO:HG2	6	1.01
(2,537)	1:8:A:TYR:HA	1:24:A:PRO:HG2	7	1.01
(2,537)	1:8:A:TYR:HA	1:24:A:PRO:HG2	8	1.01
(2,504)	1:14:A:ASP:HB3	1:19:A:SER:HB2	5	1.01
(2,459)	1:14:A:ASP:HB2	1:15:A:GLY:H	7	1.01
(2,404)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	2	1.01
(2,404)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	2	1.01
(2,252)	1:10:A:GLN:HA	1:10:A:GLN:HE21	1	1.01
(2,252)	1:10:A:GLN:HA	1:10:A:GLN:HE21	3	1.01
(1,745)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	4	1.01
(1,745)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	4	1.01
(1,545)	1:4:A:CYS:HA	1:7:A:LEU:HB3	1	1.01
(1,274)	1:11:A:TRP:H	1:12:A:LEU:HA	3	1.01
(1,95)	1:2:A:GLU:HG2	1:6:A:ARG:H	5	1.01
(2,710)	1:9:A:ILE:HA	1:12:A:LEU:HB2	5	1.0
(2,404)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	7	1.0
(2,404)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	7	1.0
(4,68)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	9	0.99
(4,68)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	9	0.99
(4,68)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	9	0.99
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG21	1	0.99
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG22	1	0.99
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG23	1	0.99
(4,13)	1:7:A:LEU:HG	1:25:A:CYS:H	9	0.99
(3,616)	1:17:A:PRO:HB2	1:18:A:SER:HB3	4	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,710)	1:9:A:ILE:HA	1:12:A:LEU:HB2	1	0.99
(2,710)	1:9:A:ILE:HA	1:12:A:LEU:HB2	4	0.99
(2,710)	1:9:A:ILE:HA	1:12:A:LEU:HB2	7	0.99
(2,575)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	3	0.99
(2,538)	1:8:A:TYR:HA	1:24:A:PRO:HG3	4	0.99
(2,436)	1:8:A:TYR:HD1	1:12:A:LEU:HG	3	0.99
(2,436)	1:8:A:TYR:HD2	1:12:A:LEU:HG	3	0.99
(2,404)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	5	0.99
(2,404)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	5	0.99
(2,242)	1:17:A:PRO:HB2	1:18:A:SER:H	6	0.99
(2,136)	1:18:A:SER:H	1:18:A:SER:HA	7	0.99
(1,711)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	9	0.99
(1,711)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	9	0.99
(1,711)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	9	0.99
(1,682)	1:17:A:PRO:HB2	1:18:A:SER:HB3	4	0.99
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG21	1	0.99
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG22	1	0.99
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG23	1	0.99
(1,252)	1:7:A:LEU:HG	1:25:A:CYS:H	9	0.99
(2,710)	1:9:A:ILE:HA	1:12:A:LEU:HB2	3	0.98
(2,694)	1:5:A:VAL:HG21	1:9:A:ILE:HB	6	0.98
(2,694)	1:5:A:VAL:HG22	1:9:A:ILE:HB	6	0.98
(2,694)	1:5:A:VAL:HG23	1:9:A:ILE:HB	6	0.98
(2,436)	1:8:A:TYR:HD1	1:12:A:LEU:HG	9	0.98
(2,436)	1:8:A:TYR:HD2	1:12:A:LEU:HG	9	0.98
(2,436)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	0.98
(2,436)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	0.98
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG2	6	0.98
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG3	6	0.98
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD11	1	0.98
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD12	1	0.98
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD13	1	0.98
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD11	7	0.98
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD12	7	0.98
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD13	7	0.98
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD11	8	0.98
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD12	8	0.98
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD13	8	0.98
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	1	0.98
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	1	0.98
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	1	0.98
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	7	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	7	0.98
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	7	0.98
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	8	0.98
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	8	0.98
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	8	0.98
(3,380)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	7	0.97
(2,710)	1:9:A:ILE:HA	1:12:A:LEU:HB2	8	0.97
(2,694)	1:5:A:VAL:HG21	1:9:A:ILE:HB	4	0.97
(2,694)	1:5:A:VAL:HG22	1:9:A:ILE:HB	4	0.97
(2,694)	1:5:A:VAL:HG23	1:9:A:ILE:HB	4	0.97
(2,538)	1:8:A:TYR:HA	1:24:A:PRO:HG3	5	0.97
(2,504)	1:14:A:ASP:HB3	1:19:A:SER:HB2	1	0.97
(2,436)	1:8:A:TYR:HD1	1:12:A:LEU:HG	6	0.97
(2,436)	1:8:A:TYR:HD2	1:12:A:LEU:HG	6	0.97
(2,223)	1:3:A:GLU:H	1:4:A:CYS:H	1	0.97
(2,184)	1:19:A:SER:HG	1:21:A:ARG:H	10	0.97
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG2	2	0.97
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG3	2	0.97
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG2	10	0.97
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG3	10	0.97
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD11	9	0.97
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD12	9	0.97
(2,20)	1:12:A:LEU:H	1:12:A:LEU:HD13	9	0.97
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD11	9	0.97
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD12	9	0.97
(2,4)	1:12:A:LEU:H	1:12:A:LEU:HD13	9	0.97
(1,408)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	7	0.97
(4,68)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	5	0.96
(4,68)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	5	0.96
(4,68)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	5	0.96
(3,630)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	7	0.96
(3,630)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	7	0.96
(3,630)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	7	0.96
(3,380)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	1	0.96
(3,91)	1:2:A:GLU:HG2	1:5:A:VAL:H	6	0.96
(2,538)	1:8:A:TYR:HA	1:24:A:PRO:HG3	10	0.96
(2,513)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	5	0.96
(2,436)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	0.96
(2,436)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	0.96
(2,436)	1:8:A:TYR:HD1	1:12:A:LEU:HG	7	0.96
(2,436)	1:8:A:TYR:HD2	1:12:A:LEU:HG	7	0.96
(2,227)	1:9:A:ILE:HB	1:11:A:TRP:H	10	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:19:A:SER:HG	1:21:A:ARG:H	9	0.96
(1,711)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	5	0.96
(1,711)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	5	0.96
(1,711)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	5	0.96
(1,697)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	7	0.96
(1,697)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	7	0.96
(1,697)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	7	0.96
(1,408)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	1	0.96
(1,96)	1:2:A:GLU:HG2	1:5:A:VAL:H	6	0.96
(4,16)	1:11:A:TRP:H	1:12:A:LEU:HA	7	0.95
(3,380)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.95
(3,91)	1:2:A:GLU:HG2	1:5:A:VAL:H	1	0.95
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	2	0.95
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	2	0.95
(2,572)	1:21:A:ARG:HD2	1:21:A:ARG:HE	6	0.95
(2,538)	1:8:A:TYR:HA	1:24:A:PRO:HG3	3	0.95
(2,537)	1:8:A:TYR:HA	1:24:A:PRO:HG2	1	0.95
(2,513)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	2	0.95
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	1	0.95
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	1	0.95
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	1	0.95
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.95
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.95
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.95
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	3	0.95
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	3	0.95
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	3	0.95
(2,404)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	3	0.95
(2,404)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	3	0.95
(1,408)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.95
(1,274)	1:11:A:TRP:H	1:12:A:LEU:HA	7	0.95
(1,96)	1:2:A:GLU:HG2	1:5:A:VAL:H	1	0.95
(4,76)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	1	0.94
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	5	0.94
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	5	0.94
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	5	0.94
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	5	0.94
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	5	0.94
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	5	0.94
(4,48)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	4	0.94
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	2	0.94
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	2	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	2	0.94
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	2	0.94
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	2	0.94
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	2	0.94
(4,12)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.94
(3,380)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	8	0.94
(2,573)	1:21:A:ARG:HD3	1:21:A:ARG:HE	7	0.94
(2,538)	1:8:A:TYR:HA	1:24:A:PRO:HG3	2	0.94
(2,538)	1:8:A:TYR:HA	1:24:A:PRO:HG3	9	0.94
(2,504)	1:14:A:ASP:HB3	1:19:A:SER:HB2	9	0.94
(2,474)	1:8:A:TYR:HD1	1:25:A:CYS:H	6	0.94
(2,474)	1:8:A:TYR:HD2	1:25:A:CYS:H	6	0.94
(2,436)	1:8:A:TYR:HD1	1:12:A:LEU:HG	2	0.94
(2,436)	1:8:A:TYR:HD2	1:12:A:LEU:HG	2	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	4	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	4	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	4	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	5	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	5	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	5	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	6	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	6	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	6	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	7	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	7	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	7	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	8	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	8	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	8	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.94
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.94
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.94
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.94
(1,743)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	1	0.94
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	5	0.94
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	5	0.94
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	5	0.94
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	5	0.94
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	5	0.94
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	5	0.94
(1,533)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	4	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	2	0.94
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	2	0.94
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	2	0.94
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	2	0.94
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	2	0.94
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	2	0.94
(1,408)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	8	0.94
(1,242)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.94
(4,68)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.93
(4,68)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.93
(4,68)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.93
(4,13)	1:7:A:LEU:HG	1:25:A:CYS:H	6	0.93
(3,380)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	3	0.93
(3,380)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	5	0.93
(3,380)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	6	0.93
(3,380)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	9	0.93
(2,573)	1:21:A:ARG:HD3	1:21:A:ARG:HE	3	0.93
(2,560)	1:6:A:ARG:HA	1:6:A:ARG:HD3	8	0.93
(2,538)	1:8:A:TYR:HA	1:24:A:PRO:HG3	7	0.93
(2,513)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	3	0.93
(2,436)	1:8:A:TYR:HD1	1:12:A:LEU:HG	4	0.93
(2,436)	1:8:A:TYR:HD2	1:12:A:LEU:HG	4	0.93
(2,436)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	0.93
(2,436)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	0.93
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	9	0.93
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	9	0.93
(2,413)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	9	0.93
(2,392)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	7	0.93
(2,392)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	7	0.93
(1,711)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.93
(1,711)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.93
(1,711)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.93
(1,408)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	3	0.93
(1,408)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	5	0.93
(1,408)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	6	0.93
(1,408)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	9	0.93
(1,252)	1:7:A:LEU:HG	1:25:A:CYS:H	6	0.93
(4,68)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	3	0.92
(4,68)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	3	0.92
(4,68)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	3	0.92
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	5	0.92
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	5	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	5	0.92
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	5	0.92
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	5	0.92
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	5	0.92
(4,25)	1:8:A:TYR:HD1	1:12:A:LEU:HA	5	0.92
(4,25)	1:8:A:TYR:HD2	1:12:A:LEU:HA	5	0.92
(3,630)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	5	0.92
(3,630)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	5	0.92
(3,630)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	5	0.92
(3,380)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	2	0.92
(3,91)	1:2:A:GLU:HG2	1:5:A:VAL:H	7	0.92
(3,91)	1:2:A:GLU:HG2	1:5:A:VAL:H	8	0.92
(2,436)	1:8:A:TYR:HD1	1:12:A:LEU:HG	1	0.92
(2,436)	1:8:A:TYR:HD2	1:12:A:LEU:HG	1	0.92
(2,392)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	8	0.92
(2,392)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	8	0.92
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG2	8	0.92
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG3	8	0.92
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.92
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.92
(1,711)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	3	0.92
(1,711)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	3	0.92
(1,711)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	3	0.92
(1,697)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	5	0.92
(1,697)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	5	0.92
(1,697)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	5	0.92
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	5	0.92
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	5	0.92
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	5	0.92
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	5	0.92
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	5	0.92
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	5	0.92
(1,408)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	2	0.92
(1,394)	1:8:A:TYR:HD1	1:12:A:LEU:HA	5	0.92
(1,394)	1:8:A:TYR:HD2	1:12:A:LEU:HA	5	0.92
(1,96)	1:2:A:GLU:HG2	1:5:A:VAL:H	7	0.92
(1,96)	1:2:A:GLU:HG2	1:5:A:VAL:H	8	0.92
(4,25)	1:8:A:TYR:HD1	1:12:A:LEU:HA	3	0.91
(4,25)	1:8:A:TYR:HD2	1:12:A:LEU:HA	3	0.91
(4,25)	1:8:A:TYR:HD1	1:12:A:LEU:HA	6	0.91
(4,25)	1:8:A:TYR:HD2	1:12:A:LEU:HA	6	0.91
(3,669)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	9	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,669)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	9	0.91
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	7	0.91
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	7	0.91
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	7	0.91
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	7	0.91
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	7	0.91
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	7	0.91
(2,574)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	10	0.91
(2,573)	1:21:A:ARG:HD3	1:21:A:ARG:HE	5	0.91
(2,513)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	6	0.91
(2,474)	1:8:A:TYR:HD1	1:25:A:CYS:H	10	0.91
(2,474)	1:8:A:TYR:HD2	1:25:A:CYS:H	10	0.91
(2,404)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	4	0.91
(2,404)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	4	0.91
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG2	7	0.91
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG3	7	0.91
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG2	9	0.91
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG3	9	0.91
(1,745)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	9	0.91
(1,745)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	9	0.91
(1,394)	1:8:A:TYR:HD1	1:12:A:LEU:HA	3	0.91
(1,394)	1:8:A:TYR:HD2	1:12:A:LEU:HA	3	0.91
(1,394)	1:8:A:TYR:HD1	1:12:A:LEU:HA	6	0.91
(1,394)	1:8:A:TYR:HD2	1:12:A:LEU:HA	6	0.91
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	9	0.9
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	9	0.9
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	9	0.9
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	9	0.9
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	9	0.9
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	9	0.9
(4,16)	1:11:A:TRP:H	1:12:A:LEU:HA	6	0.9
(4,12)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.9
(2,579)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	4	0.9
(2,538)	1:8:A:TYR:HA	1:24:A:PRO:HG3	8	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD11	2	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD12	2	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD13	2	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD21	2	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD22	2	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD23	2	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD11	4	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD12	4	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD13	4	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD21	4	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD22	4	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD23	4	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD11	5	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD12	5	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD13	5	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD21	5	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD22	5	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD23	5	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD11	7	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD12	7	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD13	7	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD21	7	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD22	7	0.9
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD23	7	0.9
(2,480)	1:19:A:SER:H	1:20:A:GLY:H	2	0.9
(2,472)	1:8:A:TYR:HD1	1:9:A:ILE:H	1	0.9
(2,472)	1:8:A:TYR:HD2	1:9:A:ILE:H	1	0.9
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	9	0.9
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	9	0.9
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	9	0.9
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	9	0.9
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	9	0.9
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	9	0.9
(1,274)	1:11:A:TRP:H	1:12:A:LEU:HA	6	0.9
(1,242)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.9
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	3	0.89
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	3	0.89
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	3	0.89
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	3	0.89
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	3	0.89
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	3	0.89
(4,25)	1:8:A:TYR:HD1	1:12:A:LEU:HA	2	0.89
(4,25)	1:8:A:TYR:HD2	1:12:A:LEU:HA	2	0.89
(4,25)	1:8:A:TYR:HD1	1:12:A:LEU:HA	4	0.89
(4,25)	1:8:A:TYR:HD2	1:12:A:LEU:HA	4	0.89
(4,16)	1:11:A:TRP:H	1:12:A:LEU:HA	8	0.89
(4,12)	1:12:A:LEU:H	1:12:A:LEU:HG	7	0.89
(4,12)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.89
(3,669)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	2	0.89
(3,669)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	2	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,572)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.89
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	1	0.89
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	1	0.89
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	1	0.89
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	1	0.89
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	1	0.89
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	1	0.89
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH21	5	0.89
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH22	5	0.89
(2,689)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	2	0.89
(2,689)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	2	0.89
(2,689)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	2	0.89
(2,648)	1:11:A:TRP:HA	1:21:A:ARG:HD2	7	0.89
(2,615)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	6	0.89
(2,615)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	6	0.89
(2,615)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	6	0.89
(2,615)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	6	0.89
(2,615)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	6	0.89
(2,615)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	6	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD11	3	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD12	3	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD13	3	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD21	3	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD22	3	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD23	3	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD11	8	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD12	8	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD13	8	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD21	8	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD22	8	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD23	8	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD11	9	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD12	9	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD13	9	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD21	9	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD22	9	0.89
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD23	9	0.89
(2,392)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	10	0.89
(2,392)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	10	0.89
(2,184)	1:19:A:SER:HG	1:21:A:ARG:H	4	0.89
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG2	3	0.89
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG3	3	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,745)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	2	0.89
(1,745)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	2	0.89
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	3	0.89
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	3	0.89
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	3	0.89
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	3	0.89
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	3	0.89
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	3	0.89
(1,631)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.89
(1,394)	1:8:A:TYR:HD1	1:12:A:LEU:HA	2	0.89
(1,394)	1:8:A:TYR:HD2	1:12:A:LEU:HA	2	0.89
(1,394)	1:8:A:TYR:HD1	1:12:A:LEU:HA	4	0.89
(1,394)	1:8:A:TYR:HD2	1:12:A:LEU:HA	4	0.89
(1,274)	1:11:A:TRP:H	1:12:A:LEU:HA	8	0.89
(1,242)	1:12:A:LEU:H	1:12:A:LEU:HG	7	0.89
(1,242)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.89
(4,68)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	2	0.88
(4,68)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	2	0.88
(4,68)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	2	0.88
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	4	0.88
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	4	0.88
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	4	0.88
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	4	0.88
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	4	0.88
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	4	0.88
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	0.88
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	0.88
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	0.88
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	0.88
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	0.88
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	0.88
(4,25)	1:8:A:TYR:HD1	1:12:A:LEU:HA	9	0.88
(4,25)	1:8:A:TYR:HD2	1:12:A:LEU:HA	9	0.88
(4,25)	1:8:A:TYR:HD1	1:12:A:LEU:HA	10	0.88
(4,25)	1:8:A:TYR:HD2	1:12:A:LEU:HA	10	0.88
(4,13)	1:7:A:LEU:HG	1:25:A:CYS:H	3	0.88
(2,560)	1:6:A:ARG:HA	1:6:A:ARG:HD3	1	0.88
(2,560)	1:6:A:ARG:HA	1:6:A:ARG:HD3	7	0.88
(2,513)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	10	0.88
(1,711)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	2	0.88
(1,711)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	2	0.88
(1,711)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	2	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	4	0.88
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	4	0.88
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	4	0.88
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	4	0.88
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	4	0.88
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	4	0.88
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	0.88
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	0.88
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	0.88
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	0.88
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	0.88
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	0.88
(1,394)	1:8:A:TYR:HD1	1:12:A:LEU:HA	9	0.88
(1,394)	1:8:A:TYR:HD2	1:12:A:LEU:HA	9	0.88
(1,394)	1:8:A:TYR:HD1	1:12:A:LEU:HA	10	0.88
(1,394)	1:8:A:TYR:HD2	1:12:A:LEU:HA	10	0.88
(1,252)	1:7:A:LEU:HG	1:25:A:CYS:H	3	0.88
(4,78)	1:5:A:VAL:HB	1:9:A:ILE:HG12	1	0.87
(4,25)	1:8:A:TYR:HD1	1:12:A:LEU:HA	7	0.87
(4,25)	1:8:A:TYR:HD2	1:12:A:LEU:HA	7	0.87
(4,25)	1:8:A:TYR:HD1	1:12:A:LEU:HA	8	0.87
(4,25)	1:8:A:TYR:HD2	1:12:A:LEU:HA	8	0.87
(4,12)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.87
(4,12)	1:12:A:LEU:H	1:12:A:LEU:HG	4	0.87
(3,669)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	3	0.87
(3,669)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	3	0.87
(3,669)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	5	0.87
(3,669)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	5	0.87
(3,669)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	10	0.87
(3,669)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	10	0.87
(3,572)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	0.87
(3,380)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	4	0.87
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	3	0.87
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	3	0.87
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	3	0.87
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	3	0.87
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	3	0.87
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	3	0.87
(2,689)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	9	0.87
(2,689)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	9	0.87
(2,689)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	9	0.87
(2,538)	1:8:A:TYR:HA	1:24:A:PRO:HG3	6	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,513)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	9	0.87
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD11	10	0.87
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD12	10	0.87
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD13	10	0.87
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD21	10	0.87
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD22	10	0.87
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD23	10	0.87
(2,401)	1:11:A:TRP:HZ3	1:23:A:PRO:HB3	6	0.87
(2,392)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	2	0.87
(2,392)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	2	0.87
(2,392)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	3	0.87
(2,392)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	3	0.87
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG2	2	0.87
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG3	2	0.87
(1,748)	1:5:A:VAL:HB	1:9:A:ILE:HG12	1	0.87
(1,745)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	3	0.87
(1,745)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	3	0.87
(1,745)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	5	0.87
(1,745)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	5	0.87
(1,745)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	10	0.87
(1,745)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	10	0.87
(1,631)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	0.87
(1,408)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	4	0.87
(1,394)	1:8:A:TYR:HD1	1:12:A:LEU:HA	7	0.87
(1,394)	1:8:A:TYR:HD2	1:12:A:LEU:HA	7	0.87
(1,394)	1:8:A:TYR:HD1	1:12:A:LEU:HA	8	0.87
(1,394)	1:8:A:TYR:HD2	1:12:A:LEU:HA	8	0.87
(1,242)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.87
(1,242)	1:12:A:LEU:H	1:12:A:LEU:HG	4	0.87
(4,50)	1:4:A:CYS:HA	1:7:A:LEU:HB3	6	0.86
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	6	0.86
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	6	0.86
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	6	0.86
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	6	0.86
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	6	0.86
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	6	0.86
(4,13)	1:7:A:LEU:HG	1:25:A:CYS:H	5	0.86
(4,12)	1:12:A:LEU:H	1:12:A:LEU:HG	3	0.86
(4,12)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.86
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	8	0.86
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	8	0.86
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	8	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	8	0.86
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	8	0.86
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	8	0.86
(2,689)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	3	0.86
(2,689)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	3	0.86
(2,689)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	3	0.86
(2,689)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	5	0.86
(2,689)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	5	0.86
(2,689)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	5	0.86
(2,689)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	10	0.86
(2,689)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	10	0.86
(2,689)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	10	0.86
(2,643)	1:8:A:TYR:H	1:10:A:GLN:H	1	0.86
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	1	0.86
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	1	0.86
(2,573)	1:21:A:ARG:HD3	1:21:A:ARG:HE	10	0.86
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD11	1	0.86
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD12	1	0.86
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD13	1	0.86
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD21	1	0.86
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD22	1	0.86
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD23	1	0.86
(2,392)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	9	0.86
(2,392)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	9	0.86
(2,155)	1:25:A:CYS:H	1:25:A:CYS:HB3	7	0.86
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG2	7	0.86
(2,107)	1:21:A:ARG:H	1:21:A:ARG:HG3	7	0.86
(1,545)	1:4:A:CYS:HA	1:7:A:LEU:HB3	6	0.86
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	6	0.86
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	6	0.86
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	6	0.86
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	6	0.86
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	6	0.86
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	6	0.86
(1,252)	1:7:A:LEU:HG	1:25:A:CYS:H	5	0.86
(1,242)	1:12:A:LEU:H	1:12:A:LEU:HG	3	0.86
(1,242)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.86
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	3	0.85
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	3	0.85
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	3	0.85
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	3	0.85
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	3	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	3	0.85
(4,16)	1:11:A:TRP:H	1:12:A:LEU:HA	5	0.85
(4,12)	1:12:A:LEU:H	1:12:A:LEU:HG	5	0.85
(4,12)	1:12:A:LEU:H	1:12:A:LEU:HG	6	0.85
(3,91)	1:2:A:GLU:HG2	1:5:A:VAL:H	5	0.85
(2,739)	1:13:A:LYS:H	1:14:A:ASP:HB3	5	0.85
(2,739)	1:13:A:LYS:H	1:14:A:ASP:HB3	8	0.85
(2,573)	1:21:A:ARG:HD3	1:21:A:ARG:HE	9	0.85
(2,538)	1:8:A:TYR:HA	1:24:A:PRO:HG3	1	0.85
(2,513)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	1	0.85
(2,513)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	8	0.85
(2,434)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.85
(2,401)	1:11:A:TRP:HZ3	1:23:A:PRO:HB3	10	0.85
(2,392)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	5	0.85
(2,392)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	5	0.85
(2,243)	1:17:A:PRO:HG2	1:18:A:SER:H	4	0.85
(2,155)	1:25:A:CYS:H	1:25:A:CYS:HB3	8	0.85
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	3	0.85
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	3	0.85
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	3	0.85
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	3	0.85
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	3	0.85
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	3	0.85
(1,274)	1:11:A:TRP:H	1:12:A:LEU:HA	5	0.85
(1,242)	1:12:A:LEU:H	1:12:A:LEU:HG	5	0.85
(1,242)	1:12:A:LEU:H	1:12:A:LEU:HG	6	0.85
(1,96)	1:2:A:GLU:HG2	1:5:A:VAL:H	5	0.85
(2,646)	1:15:A:GLY:HA2	1:19:A:SER:HB3	2	0.84
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD11	6	0.84
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD12	6	0.84
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD13	6	0.84
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD21	6	0.84
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD22	6	0.84
(2,492)	1:4:A:CYS:HA	1:7:A:LEU:HD23	6	0.84
(2,474)	1:8:A:TYR:HD1	1:25:A:CYS:H	5	0.84
(2,474)	1:8:A:TYR:HD2	1:25:A:CYS:H	5	0.84
(2,404)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	6	0.84
(2,404)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	6	0.84
(2,360)	1:11:A:TRP:HD1	1:19:A:SER:HG	9	0.84
(4,25)	1:8:A:TYR:HD1	1:12:A:LEU:HA	1	0.83
(4,25)	1:8:A:TYR:HD2	1:12:A:LEU:HA	1	0.83
(3,630)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	10	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,630)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	10	0.83
(3,630)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	10	0.83
(2,689)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	7	0.83
(2,689)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	7	0.83
(2,689)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	7	0.83
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD11	7	0.83
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD12	7	0.83
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD13	7	0.83
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD21	7	0.83
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD22	7	0.83
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD23	7	0.83
(2,656)	1:17:A:PRO:HB2	1:18:A:SER:HB3	5	0.83
(2,513)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	7	0.83
(2,474)	1:8:A:TYR:HD1	1:25:A:CYS:H	9	0.83
(2,474)	1:8:A:TYR:HD2	1:25:A:CYS:H	9	0.83
(2,441)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	4	0.83
(2,441)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	4	0.83
(2,404)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	9	0.83
(2,404)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	9	0.83
(2,401)	1:11:A:TRP:HZ3	1:23:A:PRO:HB3	9	0.83
(2,94)	1:2:A:GLU:HG2	1:6:A:ARG:H	7	0.83
(1,697)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	10	0.83
(1,697)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	10	0.83
(1,697)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	10	0.83
(1,394)	1:8:A:TYR:HD1	1:12:A:LEU:HA	1	0.83
(1,394)	1:8:A:TYR:HD2	1:12:A:LEU:HA	1	0.83
(4,50)	1:4:A:CYS:HA	1:7:A:LEU:HB3	4	0.82
(2,689)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	8	0.82
(2,689)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	8	0.82
(2,689)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	8	0.82
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD11	8	0.82
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD12	8	0.82
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD13	8	0.82
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD21	8	0.82
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD22	8	0.82
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD23	8	0.82
(2,636)	1:11:A:TRP:HE3	1:24:A:PRO:HD2	6	0.82
(2,636)	1:11:A:TRP:HE3	1:24:A:PRO:HD2	10	0.82
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB2	1	0.82
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB3	1	0.82
(2,480)	1:19:A:SER:H	1:20:A:GLY:H	5	0.82
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG21	5	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG22	5	0.82
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG23	5	0.82
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG21	5	0.82
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG22	5	0.82
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG23	5	0.82
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG2	5	0.82
(2,56)	1:3:A:GLU:H	1:3:A:GLU:HG3	5	0.82
(1,545)	1:4:A:CYS:HA	1:7:A:LEU:HB3	4	0.82
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	8	0.81
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	8	0.81
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	8	0.81
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	8	0.81
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	8	0.81
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	8	0.81
(4,16)	1:11:A:TRP:H	1:12:A:LEU:HA	9	0.81
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	6	0.81
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	6	0.81
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	6	0.81
(3,91)	1:2:A:GLU:HG2	1:5:A:VAL:H	9	0.81
(2,739)	1:13:A:LYS:H	1:14:A:ASP:HB3	7	0.81
(2,572)	1:21:A:ARG:HD2	1:21:A:ARG:HE	8	0.81
(2,474)	1:8:A:TYR:HD1	1:25:A:CYS:H	2	0.81
(2,474)	1:8:A:TYR:HD2	1:25:A:CYS:H	2	0.81
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG21	4	0.81
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG22	4	0.81
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG23	4	0.81
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG21	4	0.81
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG22	4	0.81
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG23	4	0.81
(2,401)	1:11:A:TRP:HZ3	1:23:A:PRO:HB3	3	0.81
(2,94)	1:2:A:GLU:HG2	1:6:A:ARG:H	6	0.81
(2,60)	1:4:A:CYS:H	1:4:A:CYS:HB2	6	0.81
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	6	0.81
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	6	0.81
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	6	0.81
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	8	0.81
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	8	0.81
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	8	0.81
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	8	0.81
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	8	0.81
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	8	0.81
(1,274)	1:11:A:TRP:H	1:12:A:LEU:HA	9	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:2:A:GLU:HG2	1:5:A:VAL:H	9	0.81
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	7	0.8
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	7	0.8
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	7	0.8
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	7	0.8
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	7	0.8
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	7	0.8
(3,630)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	3	0.8
(3,630)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	3	0.8
(3,630)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	3	0.8
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	5	0.8
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	5	0.8
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	5	0.8
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	5	0.8
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	5	0.8
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	5	0.8
(2,739)	1:13:A:LYS:H	1:14:A:ASP:HB3	4	0.8
(2,648)	1:11:A:TRP:HA	1:21:A:ARG:HD2	5	0.8
(2,636)	1:11:A:TRP:HE3	1:24:A:PRO:HD2	9	0.8
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	7	0.8
(2,634)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	7	0.8
(2,611)	1:19:A:SER:HB3	1:19:A:SER:HG	9	0.8
(2,560)	1:6:A:ARG:HA	1:6:A:ARG:HD3	5	0.8
(2,540)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	10	0.8
(2,540)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	10	0.8
(2,496)	1:12:A:LEU:HD21	1:13:A:LYS:HA	5	0.8
(2,496)	1:12:A:LEU:HD22	1:13:A:LYS:HA	5	0.8
(2,496)	1:12:A:LEU:HD23	1:13:A:LYS:HA	5	0.8
(2,480)	1:19:A:SER:H	1:20:A:GLY:H	1	0.8
(2,472)	1:8:A:TYR:HD1	1:9:A:ILE:H	3	0.8
(2,472)	1:8:A:TYR:HD2	1:9:A:ILE:H	3	0.8
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG21	2	0.8
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG22	2	0.8
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG23	2	0.8
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG21	2	0.8
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG22	2	0.8
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG23	2	0.8
(2,404)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	10	0.8
(2,404)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	10	0.8
(2,357)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	7	0.8
(1,697)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	3	0.8
(1,697)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	3	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	3	0.8
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	7	0.8
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	7	0.8
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	7	0.8
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	7	0.8
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	7	0.8
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	7	0.8
(2,741)	1:2:A:GLU:HA	1:5:A:VAL:H	2	0.79
(2,739)	1:13:A:LYS:H	1:14:A:ASP:HB3	3	0.79
(2,689)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	1	0.79
(2,689)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	1	0.79
(2,689)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	1	0.79
(2,689)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	4	0.79
(2,689)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	4	0.79
(2,689)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	4	0.79
(2,689)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	6	0.79
(2,689)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	6	0.79
(2,689)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	6	0.79
(2,646)	1:15:A:GLY:HA2	1:19:A:SER:HB3	1	0.79
(2,646)	1:15:A:GLY:HA2	1:19:A:SER:HB3	7	0.79
(2,575)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	4	0.79
(2,560)	1:6:A:ARG:HA	1:6:A:ARG:HD3	6	0.79
(2,401)	1:11:A:TRP:HZ3	1:23:A:PRO:HB3	5	0.79
(2,392)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	6	0.79
(2,392)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	6	0.79
(2,357)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	2	0.79
(2,357)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	8	0.79
(2,337)	1:22:A:PRO:HA	1:23:A:PRO:HG2	7	0.79
(2,245)	1:24:A:PRO:HB2	1:25:A:CYS:H	4	0.79
(2,243)	1:17:A:PRO:HG2	1:18:A:SER:H	9	0.79
(2,134)	1:18:A:SER:H	1:18:A:SER:HB2	9	0.79
(2,94)	1:2:A:GLU:HG2	1:6:A:ARG:H	1	0.79
(3,630)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	4	0.78
(3,630)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	4	0.78
(3,630)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	4	0.78
(3,91)	1:2:A:GLU:HG2	1:5:A:VAL:H	10	0.78
(2,646)	1:15:A:GLY:HA2	1:19:A:SER:HB3	3	0.78
(2,513)	1:23:A:PRO:HD3	1:24:A:PRO:HD3	4	0.78
(2,480)	1:19:A:SER:H	1:20:A:GLY:H	3	0.78
(2,189)	1:18:A:SER:H	1:19:A:SER:HB2	7	0.78
(1,697)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	4	0.78
(1,697)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	4	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	4	0.78
(1,96)	1:2:A:GLU:HG2	1:5:A:VAL:H	10	0.78
(4,46)	1:5:A:VAL:HG21	1:6:A:ARG:HA	7	0.77
(4,46)	1:5:A:VAL:HG22	1:6:A:ARG:HA	7	0.77
(4,46)	1:5:A:VAL:HG23	1:6:A:ARG:HA	7	0.77
(4,16)	1:11:A:TRP:H	1:12:A:LEU:HA	10	0.77
(3,630)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	8	0.77
(3,630)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	8	0.77
(3,630)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	8	0.77
(2,706)	1:7:A:LEU:HG	1:25:A:CYS:HB2	2	0.77
(2,706)	1:7:A:LEU:HG	1:25:A:CYS:HB2	4	0.77
(2,656)	1:17:A:PRO:HB2	1:18:A:SER:HB3	1	0.77
(2,656)	1:17:A:PRO:HB2	1:18:A:SER:HB3	2	0.77
(2,656)	1:17:A:PRO:HB2	1:18:A:SER:HB3	7	0.77
(2,646)	1:15:A:GLY:HA2	1:19:A:SER:HB3	5	0.77
(2,611)	1:19:A:SER:HB3	1:19:A:SER:HG	6	0.77
(2,611)	1:19:A:SER:HB3	1:19:A:SER:HG	7	0.77
(2,560)	1:6:A:ARG:HA	1:6:A:ARG:HD3	9	0.77
(2,540)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	8	0.77
(2,540)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	8	0.77
(2,474)	1:8:A:TYR:HD1	1:25:A:CYS:H	3	0.77
(2,474)	1:8:A:TYR:HD2	1:25:A:CYS:H	3	0.77
(2,401)	1:11:A:TRP:HZ3	1:23:A:PRO:HB3	1	0.77
(2,379)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	0.77
(2,337)	1:22:A:PRO:HA	1:23:A:PRO:HG2	8	0.77
(2,337)	1:22:A:PRO:HA	1:23:A:PRO:HG2	10	0.77
(2,154)	1:25:A:CYS:H	1:25:A:CYS:HB2	6	0.77
(1,697)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	8	0.77
(1,697)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	8	0.77
(1,697)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	8	0.77
(1,515)	1:5:A:VAL:HG21	1:6:A:ARG:HA	7	0.77
(1,515)	1:5:A:VAL:HG22	1:6:A:ARG:HA	7	0.77
(1,515)	1:5:A:VAL:HG23	1:6:A:ARG:HA	7	0.77
(1,274)	1:11:A:TRP:H	1:12:A:LEU:HA	10	0.77
(3,90)	1:2:A:GLU:HG2	1:6:A:ARG:H	2	0.76
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG2	2	0.76
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG2	2	0.76
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG2	2	0.76
(2,751)	1:12:A:LEU:HD11	1:17:A:PRO:HG3	2	0.76
(2,751)	1:12:A:LEU:HD12	1:17:A:PRO:HG3	2	0.76
(2,751)	1:12:A:LEU:HD13	1:17:A:PRO:HG3	2	0.76
(2,719)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	6	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,719)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	6	0.76
(2,679)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	2	0.76
(2,679)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	2	0.76
(2,679)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	2	0.76
(2,679)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	10	0.76
(2,679)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	10	0.76
(2,679)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	10	0.76
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD11	1	0.76
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD12	1	0.76
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD13	1	0.76
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD21	1	0.76
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD22	1	0.76
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD23	1	0.76
(2,643)	1:8:A:TYR:H	1:10:A:GLN:H	7	0.76
(2,643)	1:8:A:TYR:H	1:10:A:GLN:H	8	0.76
(2,636)	1:11:A:TRP:HE3	1:24:A:PRO:HD2	3	0.76
(2,611)	1:19:A:SER:HB3	1:19:A:SER:HG	8	0.76
(2,611)	1:19:A:SER:HB3	1:19:A:SER:HG	10	0.76
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	4	0.76
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	4	0.76
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	4	0.76
(2,502)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	9	0.76
(2,441)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	2	0.76
(2,441)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	2	0.76
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG21	8	0.76
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG22	8	0.76
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG23	8	0.76
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG21	8	0.76
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG22	8	0.76
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG23	8	0.76
(2,337)	1:22:A:PRO:HA	1:23:A:PRO:HG2	1	0.76
(2,337)	1:22:A:PRO:HA	1:23:A:PRO:HG2	9	0.76
(1,95)	1:2:A:GLU:HG2	1:6:A:ARG:H	2	0.76
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	2	0.75
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	2	0.75
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	2	0.75
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	2	0.75
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	2	0.75
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	2	0.75
(4,46)	1:5:A:VAL:HG21	1:6:A:ARG:HA	8	0.75
(4,46)	1:5:A:VAL:HG22	1:6:A:ARG:HA	8	0.75
(4,46)	1:5:A:VAL:HG23	1:6:A:ARG:HA	8	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,13)	1:7:A:LEU:HG	1:25:A:CYS:H	2	0.75
(3,372)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.75
(2,743)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	2	0.75
(2,743)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	6	0.75
(2,679)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	6	0.75
(2,679)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	6	0.75
(2,679)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	6	0.75
(2,636)	1:11:A:TRP:HE3	1:24:A:PRO:HD2	5	0.75
(2,636)	1:11:A:TRP:HE3	1:24:A:PRO:HD2	7	0.75
(2,636)	1:11:A:TRP:HE3	1:24:A:PRO:HD2	8	0.75
(2,560)	1:6:A:ARG:HA	1:6:A:ARG:HD3	3	0.75
(2,502)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	6	0.75
(2,502)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	7	0.75
(2,472)	1:8:A:TYR:HD1	1:9:A:ILE:H	6	0.75
(2,472)	1:8:A:TYR:HD2	1:9:A:ILE:H	6	0.75
(2,441)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	5	0.75
(2,441)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	5	0.75
(2,379)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	0.75
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	2	0.75
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	2	0.75
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	2	0.75
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	2	0.75
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	2	0.75
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	2	0.75
(1,515)	1:5:A:VAL:HG21	1:6:A:ARG:HA	8	0.75
(1,515)	1:5:A:VAL:HG22	1:6:A:ARG:HA	8	0.75
(1,515)	1:5:A:VAL:HG23	1:6:A:ARG:HA	8	0.75
(1,397)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.75
(1,252)	1:7:A:LEU:HG	1:25:A:CYS:H	2	0.75
(4,74)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	4	0.74
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	5	0.74
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	5	0.74
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	5	0.74
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	5	0.74
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	5	0.74
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	5	0.74
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	6	0.74
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	6	0.74
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	6	0.74
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	6	0.74
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	6	0.74
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	6	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	10	0.74
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	10	0.74
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	10	0.74
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	10	0.74
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	10	0.74
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	10	0.74
(4,51)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	10	0.74
(2,739)	1:13:A:LYS:H	1:14:A:ASP:HB3	6	0.74
(2,739)	1:13:A:LYS:H	1:14:A:ASP:HB3	9	0.74
(2,648)	1:11:A:TRP:HA	1:21:A:ARG:HD2	9	0.74
(2,646)	1:15:A:GLY:HA2	1:19:A:SER:HB3	6	0.74
(2,611)	1:19:A:SER:HB3	1:19:A:SER:HG	4	0.74
(2,472)	1:8:A:TYR:HD1	1:9:A:ILE:H	2	0.74
(2,472)	1:8:A:TYR:HD2	1:9:A:ILE:H	2	0.74
(2,472)	1:8:A:TYR:HD1	1:9:A:ILE:H	7	0.74
(2,472)	1:8:A:TYR:HD2	1:9:A:ILE:H	7	0.74
(2,401)	1:11:A:TRP:HZ3	1:23:A:PRO:HB3	2	0.74
(2,401)	1:11:A:TRP:HZ3	1:23:A:PRO:HB3	7	0.74
(2,379)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	0.74
(2,379)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	0.74
(2,379)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	0.74
(2,379)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	0.74
(2,337)	1:22:A:PRO:HA	1:23:A:PRO:HG2	5	0.74
(2,243)	1:17:A:PRO:HG2	1:18:A:SER:H	8	0.74
(1,731)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	4	0.74
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	5	0.74
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	5	0.74
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	5	0.74
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	5	0.74
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	5	0.74
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	5	0.74
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	6	0.74
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	6	0.74
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	6	0.74
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	6	0.74
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	6	0.74
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	6	0.74
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	10	0.74
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	10	0.74
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	10	0.74
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	10	0.74
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	10	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	10	0.74
(1,556)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	10	0.74
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	3	0.73
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	3	0.73
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	3	0.73
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	3	0.73
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	3	0.73
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	3	0.73
(4,50)	1:4:A:CYS:HA	1:7:A:LEU:HB3	7	0.73
(4,46)	1:5:A:VAL:HG21	1:6:A:ARG:HA	2	0.73
(4,46)	1:5:A:VAL:HG22	1:6:A:ARG:HA	2	0.73
(4,46)	1:5:A:VAL:HG23	1:6:A:ARG:HA	2	0.73
(3,372)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.73
(3,91)	1:2:A:GLU:HG2	1:5:A:VAL:H	3	0.73
(2,743)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	7	0.73
(2,743)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	8	0.73
(2,743)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	9	0.73
(2,643)	1:8:A:TYR:H	1:10:A:GLN:H	5	0.73
(2,643)	1:8:A:TYR:H	1:10:A:GLN:H	10	0.73
(2,560)	1:6:A:ARG:HA	1:6:A:ARG:HD3	4	0.73
(2,502)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	4	0.73
(2,502)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	8	0.73
(2,496)	1:12:A:LEU:HD21	1:13:A:LYS:HA	7	0.73
(2,496)	1:12:A:LEU:HD22	1:13:A:LYS:HA	7	0.73
(2,496)	1:12:A:LEU:HD23	1:13:A:LYS:HA	7	0.73
(2,401)	1:11:A:TRP:HZ3	1:23:A:PRO:HB3	8	0.73
(2,379)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	0.73
(2,379)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	0.73
(2,379)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	0.73
(2,94)	1:2:A:GLU:HG2	1:6:A:ARG:H	9	0.73
(2,60)	1:4:A:CYS:H	1:4:A:CYS:HB2	4	0.73
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	3	0.73
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	3	0.73
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	3	0.73
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	3	0.73
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	3	0.73
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	3	0.73
(1,545)	1:4:A:CYS:HA	1:7:A:LEU:HB3	7	0.73
(1,515)	1:5:A:VAL:HG21	1:6:A:ARG:HA	2	0.73
(1,515)	1:5:A:VAL:HG22	1:6:A:ARG:HA	2	0.73
(1,515)	1:5:A:VAL:HG23	1:6:A:ARG:HA	2	0.73
(1,397)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:2:A:GLU:HG2	1:5:A:VAL:H	3	0.73
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	9	0.72
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	9	0.72
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	9	0.72
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	9	0.72
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	9	0.72
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	9	0.72
(4,50)	1:4:A:CYS:HA	1:7:A:LEU:HB3	8	0.72
(4,46)	1:5:A:VAL:HG21	1:6:A:ARG:HA	3	0.72
(4,46)	1:5:A:VAL:HG22	1:6:A:ARG:HA	3	0.72
(4,46)	1:5:A:VAL:HG23	1:6:A:ARG:HA	3	0.72
(3,651)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	8	0.72
(3,651)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	8	0.72
(3,651)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	8	0.72
(3,635)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	2	0.72
(3,635)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	5	0.72
(3,600)	1:8:A:TYR:HD1	1:25:A:CYS:HB3	6	0.72
(3,600)	1:8:A:TYR:HD2	1:25:A:CYS:HB3	6	0.72
(3,372)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.72
(3,372)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.72
(3,372)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.72
(3,91)	1:2:A:GLU:HG2	1:5:A:VAL:H	2	0.72
(2,743)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	4	0.72
(2,743)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	0.72
(2,739)	1:13:A:LYS:H	1:14:A:ASP:HB3	1	0.72
(2,706)	1:7:A:LEU:HG	1:25:A:CYS:HB2	3	0.72
(2,643)	1:8:A:TYR:H	1:10:A:GLN:H	6	0.72
(2,611)	1:19:A:SER:HB3	1:19:A:SER:HG	2	0.72
(2,611)	1:19:A:SER:HB3	1:19:A:SER:HG	3	0.72
(2,611)	1:19:A:SER:HB3	1:19:A:SER:HG	5	0.72
(2,573)	1:21:A:ARG:HD3	1:21:A:ARG:HE	8	0.72
(2,560)	1:6:A:ARG:HA	1:6:A:ARG:HD3	10	0.72
(2,512)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	6	0.72
(2,512)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	10	0.72
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB2	7	0.72
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB3	7	0.72
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB2	8	0.72
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB3	8	0.72
(2,502)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	10	0.72
(2,496)	1:12:A:LEU:HD21	1:13:A:LYS:HA	8	0.72
(2,496)	1:12:A:LEU:HD22	1:13:A:LYS:HA	8	0.72
(2,496)	1:12:A:LEU:HD23	1:13:A:LYS:HA	8	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,496)	1:12:A:LEU:HD21	1:13:A:LYS:HA	9	0.72
(2,496)	1:12:A:LEU:HD22	1:13:A:LYS:HA	9	0.72
(2,496)	1:12:A:LEU:HD23	1:13:A:LYS:HA	9	0.72
(2,486)	1:15:A:GLY:H	1:16:A:GLY:H	10	0.72
(2,379)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	0.72
(2,337)	1:22:A:PRO:HA	1:23:A:PRO:HG2	3	0.72
(2,77)	1:6:A:ARG:HA	1:6:A:ARG:HG2	4	0.72
(1,723)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	8	0.72
(1,723)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	8	0.72
(1,723)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	8	0.72
(1,702)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	2	0.72
(1,702)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	5	0.72
(1,662)	1:8:A:TYR:HD1	1:25:A:CYS:HB3	6	0.72
(1,662)	1:8:A:TYR:HD2	1:25:A:CYS:HB3	6	0.72
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	9	0.72
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	9	0.72
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	9	0.72
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	9	0.72
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	9	0.72
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	9	0.72
(1,545)	1:4:A:CYS:HA	1:7:A:LEU:HB3	8	0.72
(1,515)	1:5:A:VAL:HG21	1:6:A:ARG:HA	3	0.72
(1,515)	1:5:A:VAL:HG22	1:6:A:ARG:HA	3	0.72
(1,515)	1:5:A:VAL:HG23	1:6:A:ARG:HA	3	0.72
(1,397)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.72
(1,397)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.72
(1,397)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.72
(1,96)	1:2:A:GLU:HG2	1:5:A:VAL:H	2	0.72
(4,46)	1:5:A:VAL:HG21	1:6:A:ARG:HA	9	0.71
(4,46)	1:5:A:VAL:HG22	1:6:A:ARG:HA	9	0.71
(4,46)	1:5:A:VAL:HG23	1:6:A:ARG:HA	9	0.71
(4,46)	1:5:A:VAL:HG21	1:6:A:ARG:HA	10	0.71
(4,46)	1:5:A:VAL:HG22	1:6:A:ARG:HA	10	0.71
(4,46)	1:5:A:VAL:HG23	1:6:A:ARG:HA	10	0.71
(3,630)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	1	0.71
(3,630)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	1	0.71
(3,630)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	1	0.71
(3,571)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	10	0.71
(3,372)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.71
(3,372)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.71
(3,372)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.71
(3,372)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,743)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	1	0.71
(2,743)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	3	0.71
(2,741)	1:2:A:GLU:HA	1:5:A:VAL:H	9	0.71
(2,706)	1:7:A:LEU:HG	1:25:A:CYS:HB2	7	0.71
(2,706)	1:7:A:LEU:HG	1:25:A:CYS:HB2	8	0.71
(2,643)	1:8:A:TYR:H	1:10:A:GLN:H	2	0.71
(2,636)	1:11:A:TRP:HE3	1:24:A:PRO:HD2	1	0.71
(2,636)	1:11:A:TRP:HE3	1:24:A:PRO:HD2	2	0.71
(2,611)	1:19:A:SER:HB3	1:19:A:SER:HG	1	0.71
(2,504)	1:14:A:ASP:HB3	1:19:A:SER:HB2	3	0.71
(2,496)	1:12:A:LEU:HD21	1:13:A:LYS:HA	3	0.71
(2,496)	1:12:A:LEU:HD22	1:13:A:LYS:HA	3	0.71
(2,496)	1:12:A:LEU:HD23	1:13:A:LYS:HA	3	0.71
(2,474)	1:8:A:TYR:HD1	1:25:A:CYS:H	8	0.71
(2,474)	1:8:A:TYR:HD2	1:25:A:CYS:H	8	0.71
(2,357)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	5	0.71
(2,135)	1:18:A:SER:H	1:18:A:SER:HB3	4	0.71
(1,697)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	1	0.71
(1,697)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	1	0.71
(1,697)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	1	0.71
(1,630)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	10	0.71
(1,515)	1:5:A:VAL:HG21	1:6:A:ARG:HA	9	0.71
(1,515)	1:5:A:VAL:HG22	1:6:A:ARG:HA	9	0.71
(1,515)	1:5:A:VAL:HG23	1:6:A:ARG:HA	9	0.71
(1,515)	1:5:A:VAL:HG21	1:6:A:ARG:HA	10	0.71
(1,515)	1:5:A:VAL:HG22	1:6:A:ARG:HA	10	0.71
(1,515)	1:5:A:VAL:HG23	1:6:A:ARG:HA	10	0.71
(1,397)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.71
(1,397)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.71
(1,397)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.71
(1,397)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.71
(4,46)	1:5:A:VAL:HG21	1:6:A:ARG:HA	5	0.7
(4,46)	1:5:A:VAL:HG22	1:6:A:ARG:HA	5	0.7
(4,46)	1:5:A:VAL:HG23	1:6:A:ARG:HA	5	0.7
(3,653)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	1	0.7
(3,653)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	1	0.7
(3,653)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	1	0.7
(3,653)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	1	0.7
(3,653)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	1	0.7
(3,653)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	1	0.7
(3,651)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	2	0.7
(3,651)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,651)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	2	0.7
(3,651)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	3	0.7
(3,651)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	3	0.7
(3,651)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	3	0.7
(3,635)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	9	0.7
(3,635)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	10	0.7
(3,571)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	8	0.7
(3,372)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.7
(2,743)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	5	0.7
(2,724)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	3	0.7
(2,706)	1:7:A:LEU:HG	1:25:A:CYS:HB2	5	0.7
(2,643)	1:8:A:TYR:H	1:10:A:GLN:H	3	0.7
(2,560)	1:6:A:ARG:HA	1:6:A:ARG:HD3	2	0.7
(2,502)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	2	0.7
(2,496)	1:12:A:LEU:HD21	1:13:A:LYS:HA	4	0.7
(2,496)	1:12:A:LEU:HD22	1:13:A:LYS:HA	4	0.7
(2,496)	1:12:A:LEU:HD23	1:13:A:LYS:HA	4	0.7
(2,466)	1:17:A:PRO:HA	1:18:A:SER:H	5	0.7
(2,392)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	4	0.7
(2,392)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	4	0.7
(2,357)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	1	0.7
(2,337)	1:22:A:PRO:HA	1:23:A:PRO:HG2	2	0.7
(2,337)	1:22:A:PRO:HA	1:23:A:PRO:HG2	6	0.7
(2,42)	1:13:A:LYS:HA	1:13:A:LYS:HD2	5	0.7
(1,726)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	1	0.7
(1,726)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	1	0.7
(1,726)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	1	0.7
(1,726)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	1	0.7
(1,726)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	1	0.7
(1,726)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	1	0.7
(1,723)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	2	0.7
(1,723)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	2	0.7
(1,723)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	2	0.7
(1,723)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	3	0.7
(1,723)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	3	0.7
(1,723)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	3	0.7
(1,702)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	9	0.7
(1,702)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	10	0.7
(1,630)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	8	0.7
(1,515)	1:5:A:VAL:HG21	1:6:A:ARG:HA	5	0.7
(1,515)	1:5:A:VAL:HG22	1:6:A:ARG:HA	5	0.7
(1,515)	1:5:A:VAL:HG23	1:6:A:ARG:HA	5	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.7
(4,6)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.69
(3,651)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	5	0.69
(3,651)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	5	0.69
(3,651)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	5	0.69
(3,651)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	6	0.69
(3,651)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	6	0.69
(3,651)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	6	0.69
(3,651)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	7	0.69
(3,651)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	7	0.69
(3,651)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	7	0.69
(3,651)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	9	0.69
(3,651)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	9	0.69
(3,651)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	9	0.69
(3,635)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	3	0.69
(3,375)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.69
(3,375)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	0.69
(3,375)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.69
(2,739)	1:13:A:LYS:H	1:14:A:ASP:HB3	2	0.69
(2,724)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	9	0.69
(2,643)	1:8:A:TYR:H	1:10:A:GLN:H	4	0.69
(2,643)	1:8:A:TYR:H	1:10:A:GLN:H	9	0.69
(2,636)	1:11:A:TRP:HE3	1:24:A:PRO:HD2	4	0.69
(2,573)	1:21:A:ARG:HD3	1:21:A:ARG:HE	6	0.69
(2,512)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	1	0.69
(2,512)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	3	0.69
(2,502)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	5	0.69
(2,486)	1:15:A:GLY:H	1:16:A:GLY:H	5	0.69
(2,486)	1:15:A:GLY:H	1:16:A:GLY:H	8	0.69
(2,472)	1:8:A:TYR:HD1	1:9:A:ILE:H	9	0.69
(2,472)	1:8:A:TYR:HD2	1:9:A:ILE:H	9	0.69
(2,472)	1:8:A:TYR:HD1	1:9:A:ILE:H	10	0.69
(2,472)	1:8:A:TYR:HD2	1:9:A:ILE:H	10	0.69
(2,466)	1:17:A:PRO:HA	1:18:A:SER:H	2	0.69
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	6	0.69
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	6	0.69
(2,77)	1:6:A:ARG:HA	1:6:A:ARG:HG2	10	0.69
(1,723)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	5	0.69
(1,723)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	5	0.69
(1,723)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	5	0.69
(1,723)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	6	0.69
(1,723)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	6	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,723)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	6	0.69
(1,723)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	7	0.69
(1,723)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	7	0.69
(1,723)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	7	0.69
(1,723)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	9	0.69
(1,723)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	9	0.69
(1,723)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	9	0.69
(1,702)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	3	0.69
(1,401)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.69
(1,401)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	0.69
(1,401)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.69
(1,128)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.69
(4,46)	1:5:A:VAL:HG21	1:6:A:ARG:HA	1	0.68
(4,46)	1:5:A:VAL:HG22	1:6:A:ARG:HA	1	0.68
(4,46)	1:5:A:VAL:HG23	1:6:A:ARG:HA	1	0.68
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	1	0.68
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	1	0.68
(4,33)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	1	0.68
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	1	0.68
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	1	0.68
(4,33)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	1	0.68
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.68
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.68
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.68
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.68
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.68
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.68
(4,6)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.68
(3,651)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	4	0.68
(3,651)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	4	0.68
(3,651)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	4	0.68
(3,651)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	10	0.68
(3,651)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	10	0.68
(3,651)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	10	0.68
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	1	0.68
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	1	0.68
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	1	0.68
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	4	0.68
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	4	0.68
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	4	0.68
(2,724)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	2	0.68
(2,724)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	4	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,724)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	5	0.68
(2,649)	1:5:A:VAL:HA	1:25:A:CYS:HB3	4	0.68
(2,625)	1:19:A:SER:HG	1:20:A:GLY:H	6	0.68
(2,512)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	5	0.68
(2,504)	1:14:A:ASP:HB3	1:19:A:SER:HB2	2	0.68
(2,502)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	3	0.68
(2,486)	1:15:A:GLY:H	1:16:A:GLY:H	2	0.68
(2,434)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	8	0.68
(2,275)	1:8:A:TYR:HB2	1:9:A:ILE:H	1	0.68
(2,275)	1:8:A:TYR:HB3	1:9:A:ILE:H	1	0.68
(2,155)	1:25:A:CYS:H	1:25:A:CYS:HB3	4	0.68
(2,77)	1:6:A:ARG:HA	1:6:A:ARG:HG2	3	0.68
(2,77)	1:6:A:ARG:HA	1:6:A:ARG:HG2	9	0.68
(1,723)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	4	0.68
(1,723)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	4	0.68
(1,723)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	4	0.68
(1,723)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	10	0.68
(1,723)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	10	0.68
(1,723)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	10	0.68
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	1	0.68
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	1	0.68
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	1	0.68
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	4	0.68
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	4	0.68
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	4	0.68
(1,515)	1:5:A:VAL:HG21	1:6:A:ARG:HA	1	0.68
(1,515)	1:5:A:VAL:HG22	1:6:A:ARG:HA	1	0.68
(1,515)	1:5:A:VAL:HG23	1:6:A:ARG:HA	1	0.68
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	1	0.68
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	1	0.68
(1,430)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	1	0.68
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	1	0.68
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	1	0.68
(1,430)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	1	0.68
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.68
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.68
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.68
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.68
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.68
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.68
(1,128)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.68
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	1	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	1	0.67
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	1	0.67
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	1	0.67
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	1	0.67
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	1	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD11	4	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD12	4	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD13	4	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.67
(4,6)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.67
(4,6)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.67
(4,6)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.67
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	2	0.67
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	2	0.67
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	2	0.67
(3,375)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.67
(3,375)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.67
(3,375)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.67
(3,375)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.67
(2,741)	1:2:A:GLU:HA	1:5:A:VAL:H	10	0.67
(2,724)	1:4:A:CYS:HB2	1:25:A:CYS:HB3	10	0.67
(2,706)	1:7:A:LEU:HG	1:25:A:CYS:HB2	9	0.67
(2,701)	1:8:A:TYR:HB2	1:9:A:ILE:HG12	4	0.67
(2,701)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	4	0.67
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	4	0.67
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	4	0.67
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	4	0.67
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	6	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	6	0.67
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	6	0.67
(2,580)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	8	0.67
(2,512)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	8	0.67
(2,496)	1:12:A:LEU:HD21	1:13:A:LYS:HA	10	0.67
(2,496)	1:12:A:LEU:HD22	1:13:A:LYS:HA	10	0.67
(2,496)	1:12:A:LEU:HD23	1:13:A:LYS:HA	10	0.67
(2,486)	1:15:A:GLY:H	1:16:A:GLY:H	3	0.67
(2,474)	1:8:A:TYR:HD1	1:25:A:CYS:H	7	0.67
(2,474)	1:8:A:TYR:HD2	1:25:A:CYS:H	7	0.67
(2,441)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	8	0.67
(2,441)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	8	0.67
(2,357)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	3	0.67
(2,275)	1:8:A:TYR:HB2	1:9:A:ILE:H	4	0.67
(2,275)	1:8:A:TYR:HB3	1:9:A:ILE:H	4	0.67
(2,77)	1:6:A:ARG:HA	1:6:A:ARG:HG2	5	0.67
(2,77)	1:6:A:ARG:HA	1:6:A:ARG:HG2	8	0.67
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	2	0.67
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	2	0.67
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	2	0.67
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	1	0.67
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	1	0.67
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	1	0.67
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	1	0.67
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	1	0.67
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	1	0.67
(1,401)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.67
(1,401)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.67
(1,401)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.67
(1,401)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD11	4	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD12	4	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD13	4	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.67
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.67
(1,128)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.67
(1,128)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.67
(1,128)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.67
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD11	5	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD12	5	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD13	5	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD11	8	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD12	8	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD13	8	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	0.66
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	0.66
(4,6)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.66
(4,6)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.66
(3,635)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	4	0.66
(3,375)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.66
(3,58)	1:2:A:GLU:HB3	1:4:A:CYS:H	6	0.66
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	4	0.66
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	4	0.66
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	4	0.66
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	4	0.66
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	4	0.66
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	4	0.66
(2,703)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	8	0.66
(2,512)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	9	0.66
(2,496)	1:12:A:LEU:HD21	1:13:A:LYS:HA	6	0.66
(2,496)	1:12:A:LEU:HD22	1:13:A:LYS:HA	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,496)	1:12:A:LEU:HD23	1:13:A:LYS:HA	6	0.66
(2,486)	1:15:A:GLY:H	1:16:A:GLY:H	1	0.66
(2,486)	1:15:A:GLY:H	1:16:A:GLY:H	6	0.66
(2,474)	1:8:A:TYR:HD1	1:25:A:CYS:H	1	0.66
(2,474)	1:8:A:TYR:HD2	1:25:A:CYS:H	1	0.66
(2,472)	1:8:A:TYR:HD1	1:9:A:ILE:H	5	0.66
(2,472)	1:8:A:TYR:HD2	1:9:A:ILE:H	5	0.66
(2,472)	1:8:A:TYR:HD1	1:9:A:ILE:H	8	0.66
(2,472)	1:8:A:TYR:HD2	1:9:A:ILE:H	8	0.66
(2,460)	1:24:A:PRO:HD2	1:25:A:CYS:H	10	0.66
(2,441)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	9	0.66
(2,441)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	9	0.66
(2,441)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	10	0.66
(2,441)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	10	0.66
(2,189)	1:18:A:SER:H	1:19:A:SER:HB2	6	0.66
(2,77)	1:6:A:ARG:HA	1:6:A:ARG:HG2	2	0.66
(2,77)	1:6:A:ARG:HA	1:6:A:ARG:HG2	6	0.66
(1,702)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	4	0.66
(1,401)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD11	5	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD12	5	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD13	5	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD11	8	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD12	8	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD13	8	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	0.66
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	0.66
(1,128)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.66
(1,128)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.66
(1,60)	1:2:A:GLU:HB3	1:4:A:CYS:H	6	0.66
(4,59)	1:9:A:ILE:HD11	1:10:A:GLN:H	5	0.65
(4,59)	1:9:A:ILE:HD12	1:10:A:GLN:H	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,59)	1:9:A:ILE:HD13	1:10:A:GLN:H	5	0.65
(4,50)	1:4:A:CYS:HA	1:7:A:LEU:HB3	10	0.65
(4,6)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.65
(4,6)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.65
(4,6)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.65
(3,630)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	9	0.65
(3,630)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	9	0.65
(3,630)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	9	0.65
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	8	0.65
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	8	0.65
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	8	0.65
(3,375)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	0.65
(3,375)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.65
(2,742)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	2	0.65
(2,628)	1:14:A:ASP:HB3	1:15:A:GLY:H	9	0.65
(2,580)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	10	0.65
(2,579)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	3	0.65
(2,512)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	2	0.65
(2,502)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	1	0.65
(2,460)	1:24:A:PRO:HD2	1:25:A:CYS:H	6	0.65
(2,441)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	6	0.65
(2,441)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	6	0.65
(2,275)	1:8:A:TYR:HB2	1:9:A:ILE:H	7	0.65
(2,275)	1:8:A:TYR:HB3	1:9:A:ILE:H	7	0.65
(2,77)	1:6:A:ARG:HA	1:6:A:ARG:HG2	7	0.65
(1,697)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	9	0.65
(1,697)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	9	0.65
(1,697)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	9	0.65
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	8	0.65
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	8	0.65
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	8	0.65
(1,617)	1:9:A:ILE:HD11	1:10:A:GLN:H	5	0.65
(1,617)	1:9:A:ILE:HD12	1:10:A:GLN:H	5	0.65
(1,617)	1:9:A:ILE:HD13	1:10:A:GLN:H	5	0.65
(1,545)	1:4:A:CYS:HA	1:7:A:LEU:HB3	10	0.65
(1,401)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	0.65
(1,401)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.65
(1,128)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.65
(1,128)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.65
(1,128)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.65
(4,59)	1:9:A:ILE:HD11	1:10:A:GLN:H	9	0.64
(4,59)	1:9:A:ILE:HD12	1:10:A:GLN:H	9	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,59)	1:9:A:ILE:HD13	1:10:A:GLN:H	9	0.64
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	7	0.64
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	7	0.64
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	7	0.64
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	7	0.64
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	7	0.64
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	7	0.64
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	8	0.64
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	8	0.64
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	8	0.64
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	8	0.64
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	8	0.64
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	8	0.64
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD11	7	0.64
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD12	7	0.64
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD13	7	0.64
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.64
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.64
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.64
(3,635)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	6	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	3	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	3	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	3	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	6	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	6	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	6	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	7	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	7	0.64
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	7	0.64
(2,742)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	6	0.64
(2,703)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	9	0.64
(2,679)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	1	0.64
(2,679)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	1	0.64
(2,679)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	1	0.64
(2,656)	1:17:A:PRO:HB2	1:18:A:SER:HB3	10	0.64
(2,486)	1:15:A:GLY:H	1:16:A:GLY:H	4	0.64
(2,486)	1:15:A:GLY:H	1:16:A:GLY:H	9	0.64
(2,441)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	3	0.64
(2,441)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	3	0.64
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG21	9	0.64
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG22	9	0.64
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG23	9	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG21	9	0.64
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG22	9	0.64
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG23	9	0.64
(2,357)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	9	0.64
(2,275)	1:8:A:TYR:HB2	1:9:A:ILE:H	8	0.64
(2,275)	1:8:A:TYR:HB3	1:9:A:ILE:H	8	0.64
(2,242)	1:17:A:PRO:HB2	1:18:A:SER:H	4	0.64
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG2	4	0.64
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG3	4	0.64
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	5	0.64
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	5	0.64
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	5	0.64
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	5	0.64
(2,42)	1:13:A:LYS:HA	1:13:A:LYS:HD2	6	0.64
(2,42)	1:13:A:LYS:HA	1:13:A:LYS:HD2	10	0.64
(1,702)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	6	0.64
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	3	0.64
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	3	0.64
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	3	0.64
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	6	0.64
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	6	0.64
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	6	0.64
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	7	0.64
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	7	0.64
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	7	0.64
(1,617)	1:9:A:ILE:HD11	1:10:A:GLN:H	9	0.64
(1,617)	1:9:A:ILE:HD12	1:10:A:GLN:H	9	0.64
(1,617)	1:9:A:ILE:HD13	1:10:A:GLN:H	9	0.64
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	7	0.64
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	7	0.64
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	7	0.64
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	7	0.64
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	7	0.64
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	7	0.64
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	8	0.64
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	8	0.64
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	8	0.64
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	8	0.64
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	8	0.64
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	8	0.64
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD11	7	0.64
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD12	7	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD13	7	0.64
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.64
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.64
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.64
(4,74)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	3	0.63
(4,74)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	5	0.63
(4,74)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	8	0.63
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	4	0.63
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	4	0.63
(4,55)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	4	0.63
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	4	0.63
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	4	0.63
(4,55)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	4	0.63
(3,651)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	1	0.63
(3,651)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	1	0.63
(3,651)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	1	0.63
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	9	0.63
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	9	0.63
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	9	0.63
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	10	0.63
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	10	0.63
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	10	0.63
(3,118)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.63
(2,722)	1:5:A:VAL:HB	1:9:A:ILE:HG12	8	0.63
(2,722)	1:5:A:VAL:HB	1:9:A:ILE:HG12	9	0.63
(2,579)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	2	0.63
(2,512)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	7	0.63
(2,496)	1:12:A:LEU:HD21	1:13:A:LYS:HA	1	0.63
(2,496)	1:12:A:LEU:HD22	1:13:A:LYS:HA	1	0.63
(2,496)	1:12:A:LEU:HD23	1:13:A:LYS:HA	1	0.63
(2,472)	1:8:A:TYR:HD1	1:9:A:ILE:H	4	0.63
(2,472)	1:8:A:TYR:HD2	1:9:A:ILE:H	4	0.63
(2,466)	1:17:A:PRO:HA	1:18:A:SER:H	1	0.63
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	4	0.63
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	4	0.63
(2,403)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	2	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	1	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	1	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	1	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	1	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	2	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	2	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	2	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	2	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	3	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	3	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	3	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	3	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	4	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	4	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	4	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	4	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	6	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	6	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	6	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	6	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	7	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	7	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	7	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	7	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	8	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	8	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	8	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	8	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	9	0.63
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	9	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	9	0.63
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	9	0.63
(1,731)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	3	0.63
(1,731)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	5	0.63
(1,731)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	8	0.63
(1,723)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	1	0.63
(1,723)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	1	0.63
(1,723)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	1	0.63
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	9	0.63
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	9	0.63
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	9	0.63
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	10	0.63
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	10	0.63
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	10	0.63
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	4	0.63
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	4	0.63
(1,571)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	4	0.63
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	4	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	4	0.63
(1,571)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	4	0.63
(1,123)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.63
(4,74)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	2	0.62
(4,74)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	6	0.62
(4,74)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	7	0.62
(4,74)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	9	0.62
(4,74)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	10	0.62
(4,59)	1:9:A:ILE:HD11	1:10:A:GLN:H	7	0.62
(4,59)	1:9:A:ILE:HD12	1:10:A:GLN:H	7	0.62
(4,59)	1:9:A:ILE:HD13	1:10:A:GLN:H	7	0.62
(4,59)	1:9:A:ILE:HD11	1:10:A:GLN:H	8	0.62
(4,59)	1:9:A:ILE:HD12	1:10:A:GLN:H	8	0.62
(4,59)	1:9:A:ILE:HD13	1:10:A:GLN:H	8	0.62
(4,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	4	0.62
(4,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	4	0.62
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	5	0.62
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	5	0.62
(3,626)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	5	0.62
(2,722)	1:5:A:VAL:HB	1:9:A:ILE:HG12	3	0.62
(2,722)	1:5:A:VAL:HB	1:9:A:ILE:HG12	4	0.62
(2,722)	1:5:A:VAL:HB	1:9:A:ILE:HG12	5	0.62
(2,703)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	6	0.62
(2,703)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	7	0.62
(2,703)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	10	0.62
(2,521)	1:14:A:ASP:HB2	1:16:A:GLY:H	5	0.62
(2,477)	1:18:A:SER:H	1:19:A:SER:H	10	0.62
(2,403)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	6	0.62
(2,375)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	4	0.62
(2,360)	1:11:A:TRP:HD1	1:19:A:SER:HG	10	0.62
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	3	0.62
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	3	0.62
(2,155)	1:25:A:CYS:H	1:25:A:CYS:HB3	1	0.62
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	0.62
(2,46)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	0.62
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	10	0.62
(2,46)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	10	0.62
(2,42)	1:13:A:LYS:HA	1:13:A:LYS:HD2	2	0.62
(2,42)	1:13:A:LYS:HA	1:13:A:LYS:HD2	7	0.62
(1,731)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	2	0.62
(1,731)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	6	0.62
(1,731)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	7	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,731)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	9	0.62
(1,731)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	10	0.62
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	5	0.62
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	5	0.62
(1,692)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	5	0.62
(1,617)	1:9:A:ILE:HD11	1:10:A:GLN:H	7	0.62
(1,617)	1:9:A:ILE:HD12	1:10:A:GLN:H	7	0.62
(1,617)	1:9:A:ILE:HD13	1:10:A:GLN:H	7	0.62
(1,617)	1:9:A:ILE:HD11	1:10:A:GLN:H	8	0.62
(1,617)	1:9:A:ILE:HD12	1:10:A:GLN:H	8	0.62
(1,617)	1:9:A:ILE:HD13	1:10:A:GLN:H	8	0.62
(1,439)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	4	0.62
(1,439)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	4	0.62
(3,635)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	7	0.61
(3,58)	1:2:A:GLU:HB3	1:4:A:CYS:H	4	0.61
(2,722)	1:5:A:VAL:HB	1:9:A:ILE:HG12	10	0.61
(2,706)	1:7:A:LEU:HG	1:25:A:CYS:HB2	10	0.61
(2,703)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	3	0.61
(2,679)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	3	0.61
(2,679)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	3	0.61
(2,679)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	3	0.61
(2,679)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	5	0.61
(2,679)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	5	0.61
(2,679)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	5	0.61
(2,593)	1:5:A:VAL:HG11	1:6:A:ARG:H	4	0.61
(2,593)	1:5:A:VAL:HG12	1:6:A:ARG:H	4	0.61
(2,593)	1:5:A:VAL:HG13	1:6:A:ARG:H	4	0.61
(2,579)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	5	0.61
(2,572)	1:21:A:ARG:HD2	1:21:A:ARG:HE	10	0.61
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	2	0.61
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	2	0.61
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	2	0.61
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	5	0.61
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	5	0.61
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	5	0.61
(2,441)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	7	0.61
(2,441)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	7	0.61
(2,403)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	4	0.61
(2,403)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	7	0.61
(2,275)	1:8:A:TYR:HB2	1:9:A:ILE:H	2	0.61
(2,275)	1:8:A:TYR:HB3	1:9:A:ILE:H	2	0.61
(2,77)	1:6:A:ARG:HA	1:6:A:ARG:HG2	1	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	7	0.61
(1,60)	1:2:A:GLU:HB3	1:4:A:CYS:H	4	0.61
(4,74)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	1	0.6
(4,59)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.6
(4,59)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.6
(4,59)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.6
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD11	6	0.6
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD12	6	0.6
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD13	6	0.6
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.6
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.6
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.6
(3,635)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	8	0.6
(3,596)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	1	0.6
(3,596)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	1	0.6
(3,230)	1:12:A:LEU:H	1:12:A:LEU:HB3	1	0.6
(3,230)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.6
(3,230)	1:12:A:LEU:H	1:12:A:LEU:HB3	5	0.6
(3,118)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.6
(2,703)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	4	0.6
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	3	0.6
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	3	0.6
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	3	0.6
(2,650)	1:8:A:TYR:HB2	1:25:A:CYS:HB2	6	0.6
(2,650)	1:8:A:TYR:HB3	1:25:A:CYS:HB2	6	0.6
(2,648)	1:11:A:TRP:HA	1:21:A:ARG:HD2	3	0.6
(2,579)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	1	0.6
(2,572)	1:21:A:ARG:HD2	1:21:A:ARG:HE	9	0.6
(2,429)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	2	0.6
(2,429)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	8	0.6
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG21	6	0.6
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG22	6	0.6
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG23	6	0.6
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG21	6	0.6
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG22	6	0.6
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG23	6	0.6
(2,403)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	5	0.6
(2,403)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	8	0.6
(2,357)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	6	0.6
(2,357)	1:23:A:PRO:HB3	1:24:A:PRO:HD2	10	0.6
(2,275)	1:8:A:TYR:HB2	1:9:A:ILE:H	3	0.6
(2,275)	1:8:A:TYR:HB3	1:9:A:ILE:H	3	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,245)	1:24:A:PRO:HB2	1:25:A:CYS:H	2	0.6
(2,245)	1:24:A:PRO:HB2	1:25:A:CYS:H	8	0.6
(2,154)	1:25:A:CYS:H	1:25:A:CYS:HB2	1	0.6
(1,731)	1:22:A:PRO:HB3	1:23:A:PRO:HD3	1	0.6
(1,702)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	8	0.6
(1,658)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	1	0.6
(1,658)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	1	0.6
(1,617)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.6
(1,617)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.6
(1,617)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.6
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD11	6	0.6
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD12	6	0.6
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD13	6	0.6
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.6
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.6
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.6
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB3	1	0.6
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.6
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB3	5	0.6
(1,123)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.6
(4,59)	1:9:A:ILE:HD11	1:10:A:GLN:H	4	0.59
(4,59)	1:9:A:ILE:HD12	1:10:A:GLN:H	4	0.59
(4,59)	1:9:A:ILE:HD13	1:10:A:GLN:H	4	0.59
(3,653)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	7	0.59
(3,653)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	7	0.59
(3,653)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	7	0.59
(3,653)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	7	0.59
(3,653)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	7	0.59
(3,653)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	7	0.59
(3,599)	1:8:A:TYR:HE1	1:25:A:CYS:HB3	6	0.59
(3,599)	1:8:A:TYR:HE2	1:25:A:CYS:HB3	6	0.59
(3,230)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.59
(3,230)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.59
(3,230)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.59
(3,230)	1:12:A:LEU:H	1:12:A:LEU:HB3	7	0.59
(3,230)	1:12:A:LEU:H	1:12:A:LEU:HB3	8	0.59
(2,703)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	1	0.59
(2,656)	1:17:A:PRO:HB2	1:18:A:SER:HB3	8	0.59
(2,593)	1:5:A:VAL:HG11	1:6:A:ARG:H	6	0.59
(2,593)	1:5:A:VAL:HG12	1:6:A:ARG:H	6	0.59
(2,593)	1:5:A:VAL:HG13	1:6:A:ARG:H	6	0.59
(2,579)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,486)	1:15:A:GLY:H	1:16:A:GLY:H	7	0.59
(2,460)	1:24:A:PRO:HD2	1:25:A:CYS:H	9	0.59
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	10	0.59
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	10	0.59
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG21	7	0.59
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG22	7	0.59
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG23	7	0.59
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG21	7	0.59
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG22	7	0.59
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG23	7	0.59
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG21	10	0.59
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG22	10	0.59
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG23	10	0.59
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG21	10	0.59
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG22	10	0.59
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG23	10	0.59
(2,401)	1:11:A:TRP:HZ3	1:23:A:PRO:HB3	4	0.59
(2,135)	1:18:A:SER:H	1:18:A:SER:HB3	8	0.59
(2,118)	1:11:A:TRP:HA	1:11:A:TRP:HB2	1	0.59
(2,118)	1:11:A:TRP:HA	1:11:A:TRP:HB2	3	0.59
(2,118)	1:11:A:TRP:HA	1:11:A:TRP:HB2	5	0.59
(2,118)	1:11:A:TRP:HA	1:11:A:TRP:HB2	6	0.59
(2,118)	1:11:A:TRP:HA	1:11:A:TRP:HB2	7	0.59
(2,118)	1:11:A:TRP:HA	1:11:A:TRP:HB2	8	0.59
(2,118)	1:11:A:TRP:HA	1:11:A:TRP:HB2	9	0.59
(2,118)	1:11:A:TRP:HA	1:11:A:TRP:HB2	10	0.59
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	5	0.59
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	5	0.59
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	6	0.59
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	6	0.59
(2,42)	1:13:A:LYS:HA	1:13:A:LYS:HD2	3	0.59
(1,726)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	7	0.59
(1,726)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	7	0.59
(1,726)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	7	0.59
(1,726)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	7	0.59
(1,726)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	7	0.59
(1,726)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	7	0.59
(1,661)	1:8:A:TYR:HE1	1:25:A:CYS:HB3	6	0.59
(1,661)	1:8:A:TYR:HE2	1:25:A:CYS:HB3	6	0.59
(1,617)	1:9:A:ILE:HD11	1:10:A:GLN:H	4	0.59
(1,617)	1:9:A:ILE:HD12	1:10:A:GLN:H	4	0.59
(1,617)	1:9:A:ILE:HD13	1:10:A:GLN:H	4	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.59
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.59
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.59
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB3	7	0.59
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB3	8	0.59
(4,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	8	0.58
(4,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	8	0.58
(3,596)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	6	0.58
(3,596)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	6	0.58
(3,571)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	4	0.58
(3,249)	1:19:A:SER:HB2	1:21:A:ARG:H	4	0.58
(3,230)	1:12:A:LEU:H	1:12:A:LEU:HB3	9	0.58
(3,230)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.58
(2,722)	1:5:A:VAL:HB	1:9:A:ILE:HG12	7	0.58
(2,521)	1:14:A:ASP:HB2	1:16:A:GLY:H	8	0.58
(2,496)	1:12:A:LEU:HD21	1:13:A:LYS:HA	2	0.58
(2,496)	1:12:A:LEU:HD22	1:13:A:LYS:HA	2	0.58
(2,496)	1:12:A:LEU:HD23	1:13:A:LYS:HA	2	0.58
(2,466)	1:17:A:PRO:HA	1:18:A:SER:H	3	0.58
(2,462)	1:4:A:CYS:HB3	1:5:A:VAL:H	9	0.58
(2,462)	1:4:A:CYS:HB3	1:5:A:VAL:H	10	0.58
(2,429)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	7	0.58
(2,403)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	3	0.58
(2,375)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	1	0.58
(2,375)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	9	0.58
(2,118)	1:11:A:TRP:HA	1:11:A:TRP:HB2	4	0.58
(1,658)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	6	0.58
(1,658)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	6	0.58
(1,630)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	4	0.58
(1,439)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	8	0.58
(1,439)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	8	0.58
(1,263)	1:19:A:SER:HB2	1:21:A:ARG:H	4	0.58
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB3	9	0.58
(1,241)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.58
(4,58)	1:5:A:VAL:HG21	1:6:A:ARG:H	3	0.57
(4,58)	1:5:A:VAL:HG22	1:6:A:ARG:H	3	0.57
(4,58)	1:5:A:VAL:HG23	1:6:A:ARG:H	3	0.57
(4,50)	1:4:A:CYS:HA	1:7:A:LEU:HB3	9	0.57
(4,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	5	0.57
(4,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	5	0.57
(3,653)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	4	0.57
(3,653)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,653)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	4	0.57
(3,653)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	4	0.57
(3,653)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	4	0.57
(3,653)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	4	0.57
(3,653)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	8	0.57
(3,653)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	8	0.57
(3,653)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	8	0.57
(3,653)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	8	0.57
(3,653)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	8	0.57
(3,653)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	8	0.57
(3,184)	1:18:A:SER:H	1:19:A:SER:HB2	9	0.57
(3,118)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.57
(3,118)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.57
(2,718)	1:7:A:LEU:HG	1:25:A:CYS:HB3	1	0.57
(2,701)	1:8:A:TYR:HB2	1:9:A:ILE:HG12	1	0.57
(2,701)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	1	0.57
(2,679)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	9	0.57
(2,679)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	9	0.57
(2,679)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	9	0.57
(2,654)	1:3:A:GLU:HA	1:6:A:ARG:HB2	9	0.57
(2,572)	1:21:A:ARG:HD2	1:21:A:ARG:HE	5	0.57
(2,504)	1:14:A:ASP:HB3	1:19:A:SER:HB2	4	0.57
(2,477)	1:18:A:SER:H	1:19:A:SER:H	8	0.57
(2,474)	1:8:A:TYR:HD1	1:25:A:CYS:H	4	0.57
(2,474)	1:8:A:TYR:HD2	1:25:A:CYS:H	4	0.57
(2,462)	1:4:A:CYS:HB3	1:5:A:VAL:H	2	0.57
(2,462)	1:4:A:CYS:HB3	1:5:A:VAL:H	3	0.57
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG21	3	0.57
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG22	3	0.57
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG23	3	0.57
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG21	3	0.57
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG22	3	0.57
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG23	3	0.57
(2,275)	1:8:A:TYR:HB2	1:9:A:ILE:H	6	0.57
(2,275)	1:8:A:TYR:HB3	1:9:A:ILE:H	6	0.57
(2,275)	1:8:A:TYR:HB2	1:9:A:ILE:H	9	0.57
(2,275)	1:8:A:TYR:HB3	1:9:A:ILE:H	9	0.57
(2,215)	1:21:A:ARG:HA	1:22:A:PRO:HD3	8	0.57
(2,155)	1:25:A:CYS:H	1:25:A:CYS:HB3	3	0.57
(2,118)	1:11:A:TRP:HA	1:11:A:TRP:HB2	2	0.57
(2,60)	1:4:A:CYS:H	1:4:A:CYS:HB2	9	0.57
(1,726)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,726)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	4	0.57
(1,726)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	4	0.57
(1,726)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	4	0.57
(1,726)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	4	0.57
(1,726)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	4	0.57
(1,726)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	8	0.57
(1,726)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	8	0.57
(1,726)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	8	0.57
(1,726)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	8	0.57
(1,726)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	8	0.57
(1,726)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	8	0.57
(1,615)	1:5:A:VAL:HG21	1:6:A:ARG:H	3	0.57
(1,615)	1:5:A:VAL:HG22	1:6:A:ARG:H	3	0.57
(1,615)	1:5:A:VAL:HG23	1:6:A:ARG:H	3	0.57
(1,545)	1:4:A:CYS:HA	1:7:A:LEU:HB3	9	0.57
(1,439)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	5	0.57
(1,439)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	5	0.57
(1,193)	1:18:A:SER:H	1:19:A:SER:HB2	9	0.57
(1,123)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.57
(1,123)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.57
(4,58)	1:5:A:VAL:HG21	1:6:A:ARG:H	9	0.56
(4,58)	1:5:A:VAL:HG22	1:6:A:ARG:H	9	0.56
(4,58)	1:5:A:VAL:HG23	1:6:A:ARG:H	9	0.56
(4,58)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.56
(4,58)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.56
(4,58)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.56
(4,42)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	1	0.56
(4,42)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	4	0.56
(4,42)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	5	0.56
(3,596)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	3	0.56
(3,596)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	3	0.56
(3,596)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	7	0.56
(3,596)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	7	0.56
(3,118)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.56
(3,88)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	10	0.56
(2,722)	1:5:A:VAL:HB	1:9:A:ILE:HG12	6	0.56
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	1	0.56
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	1	0.56
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	1	0.56
(2,679)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	4	0.56
(2,679)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	4	0.56
(2,679)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	4	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,678)	1:12:A:LEU:HB2	1:13:A:LYS:HD2	1	0.56
(2,678)	1:12:A:LEU:HB2	1:13:A:LYS:HD2	2	0.56
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD21	1	0.56
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD22	1	0.56
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD23	1	0.56
(2,572)	1:21:A:ARG:HD2	1:21:A:ARG:HE	3	0.56
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	3	0.56
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	3	0.56
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	3	0.56
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	9	0.56
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	9	0.56
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	9	0.56
(2,504)	1:14:A:ASP:HB3	1:19:A:SER:HB2	7	0.56
(2,484)	1:4:A:CYS:H	1:5:A:VAL:H	7	0.56
(2,465)	1:10:A:GLN:HA	1:10:A:GLN:HE22	10	0.56
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	9	0.56
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	9	0.56
(2,429)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	1	0.56
(2,275)	1:8:A:TYR:HB2	1:9:A:ILE:H	5	0.56
(2,275)	1:8:A:TYR:HB3	1:9:A:ILE:H	5	0.56
(2,192)	1:11:A:TRP:HE1	1:19:A:SER:HG	7	0.56
(2,155)	1:25:A:CYS:H	1:25:A:CYS:HB3	10	0.56
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	4	0.56
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	4	0.56
(2,60)	1:4:A:CYS:H	1:4:A:CYS:HB2	10	0.56
(2,42)	1:13:A:LYS:HA	1:13:A:LYS:HD2	1	0.56
(1,658)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	3	0.56
(1,658)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	3	0.56
(1,658)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	7	0.56
(1,658)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	7	0.56
(1,615)	1:5:A:VAL:HG21	1:6:A:ARG:H	9	0.56
(1,615)	1:5:A:VAL:HG22	1:6:A:ARG:H	9	0.56
(1,615)	1:5:A:VAL:HG23	1:6:A:ARG:H	9	0.56
(1,615)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.56
(1,615)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.56
(1,615)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.56
(1,508)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	1	0.56
(1,508)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	4	0.56
(1,508)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	5	0.56
(1,123)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.56
(1,93)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	10	0.56
(4,59)	1:9:A:ILE:HD11	1:10:A:GLN:H	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,59)	1:9:A:ILE:HD12	1:10:A:GLN:H	3	0.55
(4,59)	1:9:A:ILE:HD13	1:10:A:GLN:H	3	0.55
(4,58)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	0.55
(4,58)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	0.55
(4,58)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	0.55
(4,58)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	0.55
(4,58)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	0.55
(4,58)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	0.55
(4,42)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	2	0.55
(4,42)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	3	0.55
(4,42)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	6	0.55
(4,42)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	7	0.55
(4,42)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	9	0.55
(4,42)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	10	0.55
(4,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	2	0.55
(4,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	2	0.55
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	4	0.55
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	4	0.55
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	4	0.55
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	4	0.55
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	4	0.55
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	4	0.55
(3,118)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.55
(3,88)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	4	0.55
(3,88)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	8	0.55
(3,88)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	9	0.55
(2,701)	1:8:A:TYR:HB2	1:9:A:ILE:HG12	6	0.55
(2,701)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	6	0.55
(2,610)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	0.55
(2,579)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	7	0.55
(2,572)	1:21:A:ARG:HD2	1:21:A:ARG:HE	7	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD11	5	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD12	5	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD13	5	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD11	6	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD12	6	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD13	6	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD11	9	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD12	9	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD13	9	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD11	10	0.55
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD12	10	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD13	10	0.55
(2,510)	1:8:A:TYR:HA	1:24:A:PRO:HD2	1	0.55
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB2	10	0.55
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB3	10	0.55
(2,460)	1:24:A:PRO:HD2	1:25:A:CYS:H	3	0.55
(2,429)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	5	0.55
(2,403)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	1	0.55
(2,403)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	10	0.55
(2,387)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	4	0.55
(2,321)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	1	0.55
(2,321)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	2	0.55
(2,321)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	3	0.55
(2,321)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	5	0.55
(2,321)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	6	0.55
(2,321)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	7	0.55
(2,321)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	8	0.55
(2,321)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	10	0.55
(2,245)	1:24:A:PRO:HB2	1:25:A:CYS:H	5	0.55
(2,245)	1:24:A:PRO:HB2	1:25:A:CYS:H	7	0.55
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	5	0.55
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	5	0.55
(2,215)	1:21:A:ARG:HA	1:22:A:PRO:HD3	10	0.55
(2,155)	1:25:A:CYS:H	1:25:A:CYS:HB3	2	0.55
(2,155)	1:25:A:CYS:H	1:25:A:CYS:HB3	5	0.55
(2,155)	1:25:A:CYS:H	1:25:A:CYS:HB3	9	0.55
(2,91)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	9	0.55
(1,617)	1:9:A:ILE:HD11	1:10:A:GLN:H	3	0.55
(1,617)	1:9:A:ILE:HD12	1:10:A:GLN:H	3	0.55
(1,617)	1:9:A:ILE:HD13	1:10:A:GLN:H	3	0.55
(1,615)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	0.55
(1,615)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	0.55
(1,615)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	0.55
(1,615)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	0.55
(1,615)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	0.55
(1,615)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	0.55
(1,508)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	2	0.55
(1,508)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	3	0.55
(1,508)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	6	0.55
(1,508)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	7	0.55
(1,508)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	9	0.55
(1,508)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	10	0.55
(1,439)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	2	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	2	0.55
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	4	0.55
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	4	0.55
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	4	0.55
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	4	0.55
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	4	0.55
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	4	0.55
(1,123)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.55
(1,93)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	4	0.55
(1,93)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	8	0.55
(1,93)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	9	0.55
(4,59)	1:9:A:ILE:HD11	1:10:A:GLN:H	6	0.54
(4,59)	1:9:A:ILE:HD12	1:10:A:GLN:H	6	0.54
(4,59)	1:9:A:ILE:HD13	1:10:A:GLN:H	6	0.54
(4,58)	1:5:A:VAL:HG21	1:6:A:ARG:H	1	0.54
(4,58)	1:5:A:VAL:HG22	1:6:A:ARG:H	1	0.54
(4,58)	1:5:A:VAL:HG23	1:6:A:ARG:H	1	0.54
(4,58)	1:5:A:VAL:HG21	1:6:A:ARG:H	8	0.54
(4,58)	1:5:A:VAL:HG22	1:6:A:ARG:H	8	0.54
(4,58)	1:5:A:VAL:HG23	1:6:A:ARG:H	8	0.54
(4,50)	1:4:A:CYS:HA	1:7:A:LEU:HB3	3	0.54
(4,42)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	8	0.54
(3,596)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.54
(3,596)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.54
(3,118)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.54
(3,118)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.54
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	6	0.54
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	6	0.54
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	6	0.54
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	6	0.54
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	6	0.54
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	6	0.54
(2,722)	1:5:A:VAL:HB	1:9:A:ILE:HG12	2	0.54
(2,703)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	5	0.54
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	2	0.54
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	2	0.54
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	2	0.54
(2,586)	1:12:A:LEU:H	1:12:A:LEU:HB2	9	0.54
(2,586)	1:12:A:LEU:H	1:12:A:LEU:HB2	10	0.54
(2,575)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	5	0.54
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	10	0.54
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	10	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	10	0.54
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD11	3	0.54
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD12	3	0.54
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD13	3	0.54
(2,510)	1:8:A:TYR:HA	1:24:A:PRO:HD2	8	0.54
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB2	9	0.54
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB3	9	0.54
(2,484)	1:4:A:CYS:H	1:5:A:VAL:H	5	0.54
(2,429)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	3	0.54
(2,429)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	6	0.54
(2,387)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	2	0.54
(2,387)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	5	0.54
(2,375)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	7	0.54
(2,321)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	4	0.54
(2,321)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	9	0.54
(2,275)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.54
(2,275)	1:8:A:TYR:HB3	1:9:A:ILE:H	10	0.54
(2,192)	1:11:A:TRP:HE1	1:19:A:SER:HG	6	0.54
(2,91)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	8	0.54
(2,60)	1:4:A:CYS:H	1:4:A:CYS:HB2	3	0.54
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG2	2	0.54
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG3	2	0.54
(1,658)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	10	0.54
(1,658)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	10	0.54
(1,617)	1:9:A:ILE:HD11	1:10:A:GLN:H	6	0.54
(1,617)	1:9:A:ILE:HD12	1:10:A:GLN:H	6	0.54
(1,617)	1:9:A:ILE:HD13	1:10:A:GLN:H	6	0.54
(1,615)	1:5:A:VAL:HG21	1:6:A:ARG:H	1	0.54
(1,615)	1:5:A:VAL:HG22	1:6:A:ARG:H	1	0.54
(1,615)	1:5:A:VAL:HG23	1:6:A:ARG:H	1	0.54
(1,615)	1:5:A:VAL:HG21	1:6:A:ARG:H	8	0.54
(1,615)	1:5:A:VAL:HG22	1:6:A:ARG:H	8	0.54
(1,615)	1:5:A:VAL:HG23	1:6:A:ARG:H	8	0.54
(1,545)	1:4:A:CYS:HA	1:7:A:LEU:HB3	3	0.54
(1,508)	1:11:A:TRP:HD1	1:11:A:TRP:HZ2	8	0.54
(1,123)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.54
(1,123)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.54
(4,58)	1:5:A:VAL:HG21	1:6:A:ARG:H	7	0.53
(4,58)	1:5:A:VAL:HG22	1:6:A:ARG:H	7	0.53
(4,58)	1:5:A:VAL:HG23	1:6:A:ARG:H	7	0.53
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	2	0.53
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	2	0.53
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	2	0.53
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	2	0.53
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	2	0.53
(3,596)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	8	0.53
(3,596)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	8	0.53
(3,596)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	9	0.53
(3,596)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	9	0.53
(3,118)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.53
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	8	0.53
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	8	0.53
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	8	0.53
(2,586)	1:12:A:LEU:H	1:12:A:LEU:HB2	7	0.53
(2,579)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	9	0.53
(2,563)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	2	0.53
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD11	4	0.53
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD12	4	0.53
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD13	4	0.53
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD11	7	0.53
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD12	7	0.53
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD13	7	0.53
(2,521)	1:14:A:ASP:HB2	1:16:A:GLY:H	4	0.53
(2,511)	1:14:A:ASP:HB2	1:19:A:SER:HB2	9	0.53
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB2	3	0.53
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB3	3	0.53
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB2	5	0.53
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB3	5	0.53
(2,477)	1:18:A:SER:H	1:19:A:SER:H	7	0.53
(2,465)	1:10:A:GLN:HA	1:10:A:GLN:HE22	3	0.53
(2,445)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	7	0.53
(2,445)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	7	0.53
(2,441)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	1	0.53
(2,441)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	1	0.53
(2,433)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	4	0.53
(2,387)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	3	0.53
(2,387)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	9	0.53
(2,375)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	2	0.53
(2,375)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	3	0.53
(2,375)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	5	0.53
(2,375)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	6	0.53
(2,375)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	10	0.53
(2,360)	1:11:A:TRP:HD1	1:19:A:SER:HG	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,289)	1:12:A:LEU:HA	1:12:A:LEU:HG	4	0.53
(2,289)	1:12:A:LEU:HA	1:12:A:LEU:HG	9	0.53
(2,289)	1:12:A:LEU:HA	1:12:A:LEU:HG	10	0.53
(2,154)	1:25:A:CYS:H	1:25:A:CYS:HB2	4	0.53
(2,135)	1:18:A:SER:H	1:18:A:SER:HB3	10	0.53
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	9	0.53
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	9	0.53
(2,109)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	3	0.53
(2,91)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	4	0.53
(2,91)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	10	0.53
(1,658)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	8	0.53
(1,658)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	8	0.53
(1,658)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	9	0.53
(1,658)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	9	0.53
(1,615)	1:5:A:VAL:HG21	1:6:A:ARG:H	7	0.53
(1,615)	1:5:A:VAL:HG22	1:6:A:ARG:H	7	0.53
(1,615)	1:5:A:VAL:HG23	1:6:A:ARG:H	7	0.53
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	2	0.53
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	2	0.53
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	2	0.53
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	2	0.53
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	2	0.53
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	2	0.53
(1,123)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.53
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	8	0.52
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	8	0.52
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	8	0.52
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	8	0.52
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	8	0.52
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	8	0.52
(3,573)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	10	0.52
(3,118)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.52
(2,586)	1:12:A:LEU:H	1:12:A:LEU:HB2	4	0.52
(2,586)	1:12:A:LEU:H	1:12:A:LEU:HB2	8	0.52
(2,563)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	10	0.52
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD11	2	0.52
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD12	2	0.52
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD13	2	0.52
(2,528)	1:1:A:GLU:HA	1:1:A:GLU:HB2	10	0.52
(2,521)	1:14:A:ASP:HB2	1:16:A:GLY:H	1	0.52
(2,510)	1:8:A:TYR:HA	1:24:A:PRO:HD2	7	0.52
(2,484)	1:4:A:CYS:H	1:5:A:VAL:H	8	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,460)	1:24:A:PRO:HD2	1:25:A:CYS:H	5	0.52
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	8	0.52
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	8	0.52
(2,429)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	10	0.52
(2,387)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	1	0.52
(2,387)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	6	0.52
(2,387)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	7	0.52
(2,387)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	8	0.52
(2,387)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	0.52
(2,375)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	8	0.52
(2,245)	1:24:A:PRO:HB2	1:25:A:CYS:H	3	0.52
(2,166)	1:19:A:SER:H	1:19:A:SER:HB3	9	0.52
(2,94)	1:2:A:GLU:HG2	1:6:A:ARG:H	8	0.52
(2,94)	1:2:A:GLU:HG2	1:6:A:ARG:H	10	0.52
(2,68)	1:10:A:GLN:H	1:10:A:GLN:HB2	10	0.52
(2,42)	1:13:A:LYS:HA	1:13:A:LYS:HD2	8	0.52
(1,632)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	10	0.52
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	8	0.52
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	8	0.52
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	8	0.52
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	8	0.52
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	8	0.52
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	8	0.52
(1,123)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.52
(3,58)	1:2:A:GLU:HB3	1:4:A:CYS:H	1	0.51
(2,741)	1:2:A:GLU:HA	1:5:A:VAL:H	5	0.51
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH21	2	0.51
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH22	2	0.51
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH21	4	0.51
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH22	4	0.51
(2,701)	1:8:A:TYR:HB2	1:9:A:ILE:HG12	7	0.51
(2,701)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	7	0.51
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	5	0.51
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	5	0.51
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	5	0.51
(2,628)	1:14:A:ASP:HB3	1:15:A:GLY:H	7	0.51
(2,612)	1:19:A:SER:HB2	1:19:A:SER:HG	9	0.51
(2,586)	1:12:A:LEU:H	1:12:A:LEU:HB2	1	0.51
(2,586)	1:12:A:LEU:H	1:12:A:LEU:HB2	2	0.51
(2,586)	1:12:A:LEU:H	1:12:A:LEU:HB2	3	0.51
(2,586)	1:12:A:LEU:H	1:12:A:LEU:HB2	5	0.51
(2,586)	1:12:A:LEU:H	1:12:A:LEU:HB2	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,563)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	6	0.51
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD11	8	0.51
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD12	8	0.51
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD13	8	0.51
(2,528)	1:1:A:GLU:HA	1:1:A:GLU:HB2	6	0.51
(2,521)	1:14:A:ASP:HB2	1:16:A:GLY:H	6	0.51
(2,484)	1:4:A:CYS:H	1:5:A:VAL:H	1	0.51
(2,484)	1:4:A:CYS:H	1:5:A:VAL:H	2	0.51
(2,480)	1:19:A:SER:H	1:20:A:GLY:H	4	0.51
(2,465)	1:10:A:GLN:HA	1:10:A:GLN:HE22	4	0.51
(2,460)	1:24:A:PRO:HD2	1:25:A:CYS:H	1	0.51
(2,429)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	4	0.51
(2,403)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	9	0.51
(2,289)	1:12:A:LEU:HA	1:12:A:LEU:HG	2	0.51
(2,289)	1:12:A:LEU:HA	1:12:A:LEU:HG	7	0.51
(2,289)	1:12:A:LEU:HA	1:12:A:LEU:HG	8	0.51
(2,184)	1:19:A:SER:HG	1:21:A:ARG:H	6	0.51
(2,42)	1:13:A:LYS:HA	1:13:A:LYS:HD2	9	0.51
(1,60)	1:2:A:GLU:HB3	1:4:A:CYS:H	1	0.51
(4,59)	1:9:A:ILE:HD11	1:10:A:GLN:H	2	0.5
(4,59)	1:9:A:ILE:HD12	1:10:A:GLN:H	2	0.5
(4,59)	1:9:A:ILE:HD13	1:10:A:GLN:H	2	0.5
(4,50)	1:4:A:CYS:HA	1:7:A:LEU:HB3	5	0.5
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	5	0.5
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	5	0.5
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	5	0.5
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	5	0.5
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	5	0.5
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	5	0.5
(3,423)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	4	0.5
(3,423)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	4	0.5
(3,184)	1:18:A:SER:H	1:19:A:SER:HB2	4	0.5
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD21	2	0.5
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD22	2	0.5
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD23	2	0.5
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD21	4	0.5
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD22	4	0.5
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD23	4	0.5
(2,628)	1:14:A:ASP:HB3	1:15:A:GLY:H	1	0.5
(2,625)	1:19:A:SER:HG	1:20:A:GLY:H	2	0.5
(2,510)	1:8:A:TYR:HA	1:24:A:PRO:HD2	10	0.5
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB2	2	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB3	2	0.5
(2,465)	1:10:A:GLN:HA	1:10:A:GLN:HE22	9	0.5
(2,449)	1:8:A:TYR:HD1	1:12:A:LEU:HB3	3	0.5
(2,449)	1:8:A:TYR:HD2	1:12:A:LEU:HB3	3	0.5
(2,429)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	9	0.5
(2,289)	1:12:A:LEU:HA	1:12:A:LEU:HG	5	0.5
(2,289)	1:12:A:LEU:HA	1:12:A:LEU:HG	6	0.5
(2,246)	1:7:A:LEU:HG	1:25:A:CYS:H	10	0.5
(2,215)	1:21:A:ARG:HA	1:22:A:PRO:HD3	5	0.5
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	10	0.5
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	10	0.5
(2,94)	1:2:A:GLU:HG2	1:6:A:ARG:H	3	0.5
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG2	6	0.5
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG3	6	0.5
(1,617)	1:9:A:ILE:HD11	1:10:A:GLN:H	2	0.5
(1,617)	1:9:A:ILE:HD12	1:10:A:GLN:H	2	0.5
(1,617)	1:9:A:ILE:HD13	1:10:A:GLN:H	2	0.5
(1,545)	1:4:A:CYS:HA	1:7:A:LEU:HB3	5	0.5
(1,462)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	4	0.5
(1,462)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	4	0.5
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	5	0.5
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	5	0.5
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	5	0.5
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	5	0.5
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	5	0.5
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	5	0.5
(1,193)	1:18:A:SER:H	1:19:A:SER:HB2	4	0.5
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	5	0.49
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	5	0.49
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	5	0.49
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	5	0.49
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	5	0.49
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	5	0.49
(3,596)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	2	0.49
(3,596)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	2	0.49
(3,383)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	3	0.49
(3,383)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	3	0.49
(3,381)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	4	0.49
(3,381)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	4	0.49
(2,741)	1:2:A:GLU:HA	1:5:A:VAL:H	4	0.49
(2,719)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	4	0.49
(2,719)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,701)	1:8:A:TYR:HB2	1:9:A:ILE:HG12	8	0.49
(2,701)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	8	0.49
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD21	3	0.49
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD22	3	0.49
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD23	3	0.49
(2,563)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	3	0.49
(2,563)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	4	0.49
(2,536)	1:22:A:PRO:HB2	1:23:A:PRO:HD2	1	0.49
(2,510)	1:8:A:TYR:HA	1:24:A:PRO:HD2	2	0.49
(2,510)	1:8:A:TYR:HA	1:24:A:PRO:HD2	3	0.49
(2,465)	1:10:A:GLN:HA	1:10:A:GLN:HE22	8	0.49
(2,462)	1:4:A:CYS:HB3	1:5:A:VAL:H	4	0.49
(2,289)	1:12:A:LEU:HA	1:12:A:LEU:HG	3	0.49
(2,243)	1:17:A:PRO:HG2	1:18:A:SER:H	10	0.49
(2,215)	1:21:A:ARG:HA	1:22:A:PRO:HD3	3	0.49
(2,215)	1:21:A:ARG:HA	1:22:A:PRO:HD3	6	0.49
(2,68)	1:10:A:GLN:H	1:10:A:GLN:HB2	8	0.49
(1,658)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	2	0.49
(1,658)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	2	0.49
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	5	0.49
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	5	0.49
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	5	0.49
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	5	0.49
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	5	0.49
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	5	0.49
(1,413)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	3	0.49
(1,413)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	3	0.49
(1,410)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	4	0.49
(1,410)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	4	0.49
(3,596)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	5	0.48
(3,596)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	5	0.48
(3,383)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	0.48
(3,383)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	0.48
(3,383)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.48
(3,383)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.48
(3,58)	1:2:A:GLU:HB3	1:4:A:CYS:H	8	0.48
(3,54)	1:2:A:GLU:HB3	1:3:A:GLU:H	3	0.48
(2,717)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	6	0.48
(2,679)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	8	0.48
(2,679)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	8	0.48
(2,679)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	8	0.48
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD21	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD22	6	0.48
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD23	6	0.48
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD21	7	0.48
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD22	7	0.48
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD23	7	0.48
(2,628)	1:14:A:ASP:HB3	1:15:A:GLY:H	2	0.48
(2,628)	1:14:A:ASP:HB3	1:15:A:GLY:H	5	0.48
(2,618)	1:6:A:ARG:HA	1:8:A:TYR:H	8	0.48
(2,572)	1:21:A:ARG:HD2	1:21:A:ARG:HE	1	0.48
(2,572)	1:21:A:ARG:HD2	1:21:A:ARG:HE	4	0.48
(2,563)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	5	0.48
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD11	1	0.48
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD12	1	0.48
(2,551)	1:11:A:TRP:HB3	1:12:A:LEU:HD13	1	0.48
(2,536)	1:22:A:PRO:HB2	1:23:A:PRO:HD2	3	0.48
(2,536)	1:22:A:PRO:HB2	1:23:A:PRO:HD2	9	0.48
(2,510)	1:8:A:TYR:HA	1:24:A:PRO:HD2	5	0.48
(2,465)	1:10:A:GLN:HA	1:10:A:GLN:HE22	2	0.48
(2,462)	1:4:A:CYS:HB3	1:5:A:VAL:H	5	0.48
(2,449)	1:8:A:TYR:HD1	1:12:A:LEU:HB3	5	0.48
(2,449)	1:8:A:TYR:HD2	1:12:A:LEU:HB3	5	0.48
(2,445)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	3	0.48
(2,445)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	3	0.48
(2,445)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	8	0.48
(2,445)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	8	0.48
(2,426)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	2	0.48
(2,426)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	2	0.48
(2,245)	1:24:A:PRO:HB2	1:25:A:CYS:H	1	0.48
(2,166)	1:19:A:SER:H	1:19:A:SER:HB3	8	0.48
(2,134)	1:18:A:SER:H	1:18:A:SER:HB2	4	0.48
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	1	0.48
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	1	0.48
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	2	0.48
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	2	0.48
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	8	0.48
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	8	0.48
(2,68)	1:10:A:GLN:H	1:10:A:GLN:HB2	9	0.48
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG2	10	0.48
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG3	10	0.48
(1,658)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	5	0.48
(1,658)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	5	0.48
(1,413)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	0.48
(1,413)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.48
(1,413)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.48
(1,60)	1:2:A:GLU:HB3	1:4:A:CYS:H	8	0.48
(1,56)	1:2:A:GLU:HB3	1:3:A:GLU:H	3	0.48
(4,58)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	0.47
(4,58)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	0.47
(4,58)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	0.47
(4,50)	1:4:A:CYS:HA	1:7:A:LEU:HB3	2	0.47
(3,423)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	8	0.47
(3,423)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	8	0.47
(3,383)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	4	0.47
(3,383)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	4	0.47
(3,383)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	6	0.47
(3,383)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	6	0.47
(3,54)	1:2:A:GLU:HB3	1:3:A:GLU:H	4	0.47
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	7	0.47
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	7	0.47
(2,703)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	2	0.47
(2,679)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	7	0.47
(2,679)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	7	0.47
(2,679)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	7	0.47
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD21	8	0.47
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD22	8	0.47
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD23	8	0.47
(2,647)	1:11:A:TRP:HA	1:21:A:ARG:HD3	6	0.47
(2,628)	1:14:A:ASP:HB3	1:15:A:GLY:H	3	0.47
(2,625)	1:19:A:SER:HG	1:20:A:GLY:H	1	0.47
(2,618)	1:6:A:ARG:HA	1:8:A:TYR:H	1	0.47
(2,618)	1:6:A:ARG:HA	1:8:A:TYR:H	7	0.47
(2,612)	1:19:A:SER:HB2	1:19:A:SER:HG	7	0.47
(2,572)	1:21:A:ARG:HD2	1:21:A:ARG:HE	2	0.47
(2,563)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	7	0.47
(2,528)	1:1:A:GLU:HA	1:1:A:GLU:HB2	7	0.47
(2,510)	1:8:A:TYR:HA	1:24:A:PRO:HD2	9	0.47
(2,449)	1:8:A:TYR:HD1	1:12:A:LEU:HB3	6	0.47
(2,449)	1:8:A:TYR:HD2	1:12:A:LEU:HB3	6	0.47
(2,449)	1:8:A:TYR:HD1	1:12:A:LEU:HB3	9	0.47
(2,449)	1:8:A:TYR:HD2	1:12:A:LEU:HB3	9	0.47
(2,449)	1:8:A:TYR:HD1	1:12:A:LEU:HB3	10	0.47
(2,449)	1:8:A:TYR:HD2	1:12:A:LEU:HB3	10	0.47
(2,433)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,433)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	6	0.47
(2,268)	1:11:A:TRP:H	1:12:A:LEU:HA	2	0.47
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	2	0.47
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	2	0.47
(2,215)	1:21:A:ARG:HA	1:22:A:PRO:HD3	1	0.47
(2,215)	1:21:A:ARG:HA	1:22:A:PRO:HD3	2	0.47
(2,154)	1:25:A:CYS:H	1:25:A:CYS:HB2	2	0.47
(2,109)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	7	0.47
(2,95)	1:2:A:GLU:HG2	1:5:A:VAL:H	6	0.47
(2,68)	1:10:A:GLN:H	1:10:A:GLN:HB2	4	0.47
(2,60)	1:4:A:CYS:H	1:4:A:CYS:HB2	5	0.47
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG2	1	0.47
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG3	1	0.47
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG2	3	0.47
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG3	3	0.47
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG2	8	0.47
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG3	8	0.47
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG2	9	0.47
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG3	9	0.47
(1,615)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	0.47
(1,615)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	0.47
(1,615)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	0.47
(1,545)	1:4:A:CYS:HA	1:7:A:LEU:HB3	2	0.47
(1,462)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	8	0.47
(1,462)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	8	0.47
(1,413)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	4	0.47
(1,413)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	4	0.47
(1,413)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	6	0.47
(1,413)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	6	0.47
(1,56)	1:2:A:GLU:HB3	1:3:A:GLU:H	4	0.47
(4,64)	1:5:A:VAL:HA	1:25:A:CYS:HB3	5	0.46
(4,59)	1:9:A:ILE:HD11	1:10:A:GLN:H	1	0.46
(4,59)	1:9:A:ILE:HD12	1:10:A:GLN:H	1	0.46
(4,59)	1:9:A:ILE:HD13	1:10:A:GLN:H	1	0.46
(4,58)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.46
(4,58)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.46
(4,58)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.46
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.46
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.46
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.46
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.46
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,18)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.46
(3,572)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	0.46
(3,423)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	5	0.46
(3,423)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	5	0.46
(3,54)	1:2:A:GLU:HB3	1:3:A:GLU:H	5	0.46
(3,54)	1:2:A:GLU:HB3	1:3:A:GLU:H	9	0.46
(3,54)	1:2:A:GLU:HB3	1:3:A:GLU:H	10	0.46
(2,701)	1:8:A:TYR:HB2	1:9:A:ILE:HG12	9	0.46
(2,701)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	9	0.46
(2,678)	1:12:A:LEU:HB2	1:13:A:LYS:HD2	8	0.46
(2,628)	1:14:A:ASP:HB3	1:15:A:GLY:H	4	0.46
(2,625)	1:19:A:SER:HG	1:20:A:GLY:H	5	0.46
(2,618)	1:6:A:ARG:HA	1:8:A:TYR:H	3	0.46
(2,563)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	9	0.46
(2,536)	1:22:A:PRO:HB2	1:23:A:PRO:HD2	7	0.46
(2,528)	1:1:A:GLU:HA	1:1:A:GLU:HB2	5	0.46
(2,521)	1:14:A:ASP:HB2	1:16:A:GLY:H	2	0.46
(2,521)	1:14:A:ASP:HB2	1:16:A:GLY:H	9	0.46
(2,480)	1:19:A:SER:H	1:20:A:GLY:H	7	0.46
(2,460)	1:24:A:PRO:HD2	1:25:A:CYS:H	2	0.46
(2,460)	1:24:A:PRO:HD2	1:25:A:CYS:H	7	0.46
(2,460)	1:24:A:PRO:HD2	1:25:A:CYS:H	8	0.46
(2,449)	1:8:A:TYR:HD1	1:12:A:LEU:HB3	2	0.46
(2,449)	1:8:A:TYR:HD2	1:12:A:LEU:HB3	2	0.46
(2,449)	1:8:A:TYR:HD1	1:12:A:LEU:HB3	4	0.46
(2,449)	1:8:A:TYR:HD2	1:12:A:LEU:HB3	4	0.46
(2,445)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	9	0.46
(2,445)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	9	0.46
(2,433)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	7	0.46
(2,289)	1:12:A:LEU:HA	1:12:A:LEU:HG	1	0.46
(2,95)	1:2:A:GLU:HG2	1:5:A:VAL:H	1	0.46
(1,675)	1:5:A:VAL:HA	1:25:A:CYS:HB3	5	0.46
(1,631)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	0.46
(1,617)	1:9:A:ILE:HD11	1:10:A:GLN:H	1	0.46
(1,617)	1:9:A:ILE:HD12	1:10:A:GLN:H	1	0.46
(1,617)	1:9:A:ILE:HD13	1:10:A:GLN:H	1	0.46
(1,615)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.46
(1,615)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.46
(1,615)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.46
(1,462)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	5	0.46
(1,462)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	5	0.46
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.46
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.46
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.46
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.46
(1,287)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.46
(1,56)	1:2:A:GLU:HB3	1:3:A:GLU:H	5	0.46
(1,56)	1:2:A:GLU:HB3	1:3:A:GLU:H	9	0.46
(1,56)	1:2:A:GLU:HB3	1:3:A:GLU:H	10	0.46
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	2	0.45
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	2	0.45
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	2	0.45
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	2	0.45
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	2	0.45
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	2	0.45
(3,572)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	0.45
(3,572)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	7	0.45
(3,381)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	6	0.45
(3,381)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	6	0.45
(3,54)	1:2:A:GLU:HB3	1:3:A:GLU:H	2	0.45
(3,54)	1:2:A:GLU:HB3	1:3:A:GLU:H	6	0.45
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	5	0.45
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	5	0.45
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	5	0.45
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	5	0.45
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	5	0.45
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	5	0.45
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD21	5	0.45
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD22	5	0.45
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD23	5	0.45
(2,654)	1:3:A:GLU:HA	1:6:A:ARG:HB2	3	0.45
(2,618)	1:6:A:ARG:HA	1:8:A:TYR:H	5	0.45
(2,582)	1:7:A:LEU:HG	1:8:A:TYR:H	4	0.45
(2,582)	1:7:A:LEU:HG	1:8:A:TYR:H	6	0.45
(2,563)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	1	0.45
(2,536)	1:22:A:PRO:HB2	1:23:A:PRO:HD2	6	0.45
(2,536)	1:22:A:PRO:HB2	1:23:A:PRO:HD2	10	0.45
(2,528)	1:1:A:GLU:HA	1:1:A:GLU:HB2	4	0.45
(2,528)	1:1:A:GLU:HA	1:1:A:GLU:HB2	9	0.45
(2,510)	1:8:A:TYR:HA	1:24:A:PRO:HD2	6	0.45
(2,484)	1:4:A:CYS:H	1:5:A:VAL:H	3	0.45
(2,465)	1:10:A:GLN:HA	1:10:A:GLN:HE22	6	0.45
(2,449)	1:8:A:TYR:HD1	1:12:A:LEU:HB3	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,449)	1:8:A:TYR:HD2	1:12:A:LEU:HB3	1	0.45
(2,426)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	5	0.45
(2,426)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	5	0.45
(2,426)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	8	0.45
(2,426)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	8	0.45
(2,215)	1:21:A:ARG:HA	1:22:A:PRO:HD3	7	0.45
(2,166)	1:19:A:SER:H	1:19:A:SER:HB3	4	0.45
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	7	0.45
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	7	0.45
(2,109)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	2	0.45
(2,94)	1:2:A:GLU:HG2	1:6:A:ARG:H	5	0.45
(2,68)	1:10:A:GLN:H	1:10:A:GLN:HB2	6	0.45
(2,60)	1:4:A:CYS:H	1:4:A:CYS:HB2	2	0.45
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG2	4	0.45
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG3	4	0.45
(2,42)	1:13:A:LYS:HA	1:13:A:LYS:HD2	4	0.45
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	2	0.45
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	2	0.45
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	2	0.45
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	2	0.45
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	2	0.45
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	2	0.45
(1,631)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	0.45
(1,631)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	7	0.45
(1,410)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	6	0.45
(1,410)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	6	0.45
(1,56)	1:2:A:GLU:HB3	1:3:A:GLU:H	2	0.45
(1,56)	1:2:A:GLU:HB3	1:3:A:GLU:H	6	0.45
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	2	0.44
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	2	0.44
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	2	0.44
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	2	0.44
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	2	0.44
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	2	0.44
(4,38)	1:11:A:TRP:HE3	1:12:A:LEU:HG	7	0.44
(4,13)	1:7:A:LEU:HG	1:25:A:CYS:H	4	0.44
(4,13)	1:7:A:LEU:HG	1:25:A:CYS:H	7	0.44
(3,383)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	7	0.44
(3,383)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	7	0.44
(3,54)	1:2:A:GLU:HB3	1:3:A:GLU:H	1	0.44
(2,701)	1:8:A:TYR:HB2	1:9:A:ILE:HG12	5	0.44
(2,701)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	8	0.44
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	8	0.44
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	8	0.44
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	8	0.44
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	8	0.44
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	8	0.44
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	10	0.44
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	10	0.44
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	10	0.44
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	1	0.44
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	1	0.44
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	1	0.44
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD11	1	0.44
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD12	1	0.44
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD13	1	0.44
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	4	0.44
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	4	0.44
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	4	0.44
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD11	4	0.44
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD12	4	0.44
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD13	4	0.44
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD21	9	0.44
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD22	9	0.44
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD23	9	0.44
(2,650)	1:8:A:TYR:HB2	1:25:A:CYS:HB2	1	0.44
(2,650)	1:8:A:TYR:HB3	1:25:A:CYS:HB2	1	0.44
(2,618)	1:6:A:ARG:HA	1:8:A:TYR:H	10	0.44
(2,536)	1:22:A:PRO:HB2	1:23:A:PRO:HD2	8	0.44
(2,521)	1:14:A:ASP:HB2	1:16:A:GLY:H	3	0.44
(2,480)	1:19:A:SER:H	1:20:A:GLY:H	9	0.44
(2,465)	1:10:A:GLN:HA	1:10:A:GLN:HE22	1	0.44
(2,449)	1:8:A:TYR:HD1	1:12:A:LEU:HB3	7	0.44
(2,449)	1:8:A:TYR:HD2	1:12:A:LEU:HB3	7	0.44
(2,449)	1:8:A:TYR:HD1	1:12:A:LEU:HB3	8	0.44
(2,449)	1:8:A:TYR:HD2	1:12:A:LEU:HB3	8	0.44
(2,445)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	10	0.44
(2,445)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	10	0.44
(2,433)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	9	0.44
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	1	0.44
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	1	0.44
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	1	0.44
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	1	0.44
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	1	0.44
(2,363)	1:11:A:TRP:HZ2	1:22:A:PRO:HA	1	0.44
(2,268)	1:11:A:TRP:H	1:12:A:LEU:HA	1	0.44
(2,245)	1:24:A:PRO:HB2	1:25:A:CYS:H	9	0.44
(2,142)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	3	0.44
(2,142)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	7	0.44
(2,102)	1:21:A:ARG:H	1:21:A:ARG:HD2	5	0.44
(2,99)	1:21:A:ARG:HA	1:21:A:ARG:HB3	9	0.44
(2,68)	1:10:A:GLN:H	1:10:A:GLN:HB2	5	0.44
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG2	7	0.44
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG3	7	0.44
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	2	0.44
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	2	0.44
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	2	0.44
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	2	0.44
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	2	0.44
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	2	0.44
(1,450)	1:11:A:TRP:HE3	1:12:A:LEU:HG	7	0.44
(1,413)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	7	0.44
(1,413)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	7	0.44
(1,252)	1:7:A:LEU:HG	1:25:A:CYS:H	4	0.44
(1,252)	1:7:A:LEU:HG	1:25:A:CYS:H	7	0.44
(1,56)	1:2:A:GLU:HB3	1:3:A:GLU:H	1	0.44
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	10	0.43
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	10	0.43
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	10	0.43
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	10	0.43
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	10	0.43
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	10	0.43
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG21	7	0.43
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG22	7	0.43
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG23	7	0.43
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG21	8	0.43
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG22	8	0.43
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG23	8	0.43
(4,38)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.43
(4,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	7	0.43
(4,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	7	0.43
(4,13)	1:7:A:LEU:HG	1:25:A:CYS:H	8	0.43
(4,3)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.43
(3,576)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,572)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	0.43
(3,572)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	6	0.43
(3,519)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	6	0.43
(3,423)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	2	0.43
(3,423)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	2	0.43
(3,383)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	1	0.43
(3,383)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	1	0.43
(3,108)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	4	0.43
(3,54)	1:2:A:GLU:HB3	1:3:A:GLU:H	7	0.43
(3,54)	1:2:A:GLU:HB3	1:3:A:GLU:H	8	0.43
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	6	0.43
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	6	0.43
(2,701)	1:8:A:TYR:HB2	1:9:A:ILE:HG12	2	0.43
(2,701)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	2	0.43
(2,701)	1:8:A:TYR:HB2	1:9:A:ILE:HG12	3	0.43
(2,701)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	3	0.43
(2,701)	1:8:A:TYR:HB2	1:9:A:ILE:HG12	10	0.43
(2,701)	1:8:A:TYR:HB3	1:9:A:ILE:HG12	10	0.43
(2,671)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	7	0.43
(2,671)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	7	0.43
(2,671)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	7	0.43
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD21	10	0.43
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD22	10	0.43
(2,663)	1:9:A:ILE:HA	1:12:A:LEU:HD23	10	0.43
(2,612)	1:19:A:SER:HB2	1:19:A:SER:HG	6	0.43
(2,563)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	8	0.43
(2,536)	1:22:A:PRO:HB2	1:23:A:PRO:HD2	5	0.43
(2,495)	1:5:A:VAL:HG11	1:6:A:ARG:HA	6	0.43
(2,495)	1:5:A:VAL:HG12	1:6:A:ARG:HA	6	0.43
(2,495)	1:5:A:VAL:HG13	1:6:A:ARG:HA	6	0.43
(2,480)	1:19:A:SER:H	1:20:A:GLY:H	8	0.43
(2,477)	1:18:A:SER:H	1:19:A:SER:H	4	0.43
(2,438)	1:8:A:TYR:HE1	1:23:A:PRO:HG3	4	0.43
(2,438)	1:8:A:TYR:HE2	1:23:A:PRO:HG3	4	0.43
(2,402)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	1	0.43
(2,402)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	1	0.43
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	4	0.43
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	4	0.43
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	4	0.43
(2,278)	1:7:A:LEU:HA	1:7:A:LEU:HB3	1	0.43
(2,268)	1:11:A:TRP:H	1:12:A:LEU:HA	4	0.43
(2,215)	1:21:A:ARG:HA	1:22:A:PRO:HD3	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	1:25:A:CYS:H	1:25:A:CYS:HB2	5	0.43
(2,142)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	1	0.43
(2,142)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	2	0.43
(2,142)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	4	0.43
(2,142)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	5	0.43
(2,142)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	6	0.43
(2,142)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	8	0.43
(2,142)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	9	0.43
(2,109)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	5	0.43
(2,99)	1:21:A:ARG:HA	1:21:A:ARG:HB3	5	0.43
(2,95)	1:2:A:GLU:HG2	1:5:A:VAL:H	7	0.43
(2,95)	1:2:A:GLU:HG2	1:5:A:VAL:H	8	0.43
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	10	0.43
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	10	0.43
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	10	0.43
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	10	0.43
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	10	0.43
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	10	0.43
(1,635)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	4	0.43
(1,631)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	0.43
(1,631)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	6	0.43
(1,575)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	6	0.43
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG21	7	0.43
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG22	7	0.43
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG23	7	0.43
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG21	8	0.43
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG22	8	0.43
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG23	8	0.43
(1,462)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	2	0.43
(1,462)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	2	0.43
(1,450)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.43
(1,439)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	7	0.43
(1,439)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	7	0.43
(1,413)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	1	0.43
(1,413)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	1	0.43
(1,252)	1:7:A:LEU:HG	1:25:A:CYS:H	8	0.43
(1,113)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	4	0.43
(1,75)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.43
(1,56)	1:2:A:GLU:HB3	1:3:A:GLU:H	7	0.43
(1,56)	1:2:A:GLU:HB3	1:3:A:GLU:H	8	0.43
(4,79)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	2	0.42
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	6	0.42
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	6	0.42
(4,72)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	6	0.42
(4,72)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	6	0.42
(4,72)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	6	0.42
(4,64)	1:5:A:VAL:HA	1:25:A:CYS:HB3	9	0.42
(4,64)	1:5:A:VAL:HA	1:25:A:CYS:HB3	10	0.42
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	3	0.42
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	3	0.42
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	3	0.42
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	3	0.42
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	3	0.42
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	3	0.42
(4,38)	1:11:A:TRP:HE3	1:12:A:LEU:HG	9	0.42
(4,38)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.42
(4,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	1	0.42
(4,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	1	0.42
(4,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	6	0.42
(4,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	6	0.42
(4,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	9	0.42
(4,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	9	0.42
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	9	0.42
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	9	0.42
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	9	0.42
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	10	0.42
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	10	0.42
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	10	0.42
(3,668)	1:7:A:LEU:HG	1:25:A:CYS:HB3	6	0.42
(3,572)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	0.42
(3,519)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	10	0.42
(2,706)	1:7:A:LEU:HG	1:25:A:CYS:HB2	6	0.42
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	4	0.42
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	4	0.42
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	4	0.42
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	4	0.42
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	4	0.42
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	4	0.42
(2,656)	1:17:A:PRO:HB2	1:18:A:SER:HB3	9	0.42
(2,654)	1:3:A:GLU:HA	1:6:A:ARG:HB2	5	0.42
(2,618)	1:6:A:ARG:HA	1:8:A:TYR:H	9	0.42
(2,557)	1:23:A:PRO:HA	1:24:A:PRO:HD2	8	0.42
(2,527)	1:1:A:GLU:HA	1:1:A:GLU:HG2	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,527)	1:1:A:GLU:HA	1:1:A:GLU:HG3	9	0.42
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	2	0.42
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	2	0.42
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	2	0.42
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	3	0.42
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	3	0.42
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	3	0.42
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	9	0.42
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	9	0.42
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	9	0.42
(2,268)	1:11:A:TRP:H	1:12:A:LEU:HA	3	0.42
(2,166)	1:19:A:SER:H	1:19:A:SER:HB3	10	0.42
(2,142)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.42
(2,134)	1:18:A:SER:H	1:18:A:SER:HB2	8	0.42
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	3	0.42
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	3	0.42
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	3	0.42
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	3	0.42
(2,109)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	1	0.42
(2,99)	1:21:A:ARG:HA	1:21:A:ARG:HB3	7	0.42
(2,68)	1:10:A:GLN:H	1:10:A:GLN:HB2	1	0.42
(2,68)	1:10:A:GLN:H	1:10:A:GLN:HB2	7	0.42
(1,749)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	2	0.42
(1,744)	1:7:A:LEU:HG	1:25:A:CYS:HB3	6	0.42
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	6	0.42
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	6	0.42
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	6	0.42
(1,722)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	6	0.42
(1,722)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	6	0.42
(1,722)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	6	0.42
(1,675)	1:5:A:VAL:HA	1:25:A:CYS:HB3	9	0.42
(1,675)	1:5:A:VAL:HA	1:25:A:CYS:HB3	10	0.42
(1,631)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	0.42
(1,575)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	10	0.42
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	3	0.42
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	3	0.42
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	3	0.42
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	3	0.42
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	3	0.42
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	3	0.42
(1,450)	1:11:A:TRP:HE3	1:12:A:LEU:HG	9	0.42
(1,450)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	1	0.42
(1,439)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	1	0.42
(1,439)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	6	0.42
(1,439)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	6	0.42
(1,439)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	9	0.42
(1,439)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	9	0.42
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	9	0.42
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	9	0.42
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	9	0.42
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	10	0.42
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	10	0.42
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	10	0.42
(4,68)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	0.41
(4,68)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	0.41
(4,68)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	0.41
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	6	0.41
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	6	0.41
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	6	0.41
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	6	0.41
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	6	0.41
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	6	0.41
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.41
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.41
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.41
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	10	0.41
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	10	0.41
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	10	0.41
(4,38)	1:11:A:TRP:HE3	1:12:A:LEU:HG	1	0.41
(4,38)	1:11:A:TRP:HE3	1:12:A:LEU:HG	5	0.41
(4,38)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	0.41
(4,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	3	0.41
(4,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	3	0.41
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	2	0.41
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	2	0.41
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	2	0.41
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	5	0.41
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	5	0.41
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	5	0.41
(3,657)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	2	0.41
(3,596)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	4	0.41
(3,596)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	4	0.41
(3,573)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,573)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	9	0.41
(3,519)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	3	0.41
(3,519)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	9	0.41
(3,424)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	5	0.41
(3,424)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	7	0.41
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	9	0.41
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	9	0.41
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	9	0.41
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	9	0.41
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	9	0.41
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	9	0.41
(2,678)	1:12:A:LEU:HB2	1:13:A:LYS:HD2	3	0.41
(2,600)	1:11:A:TRP:H	1:11:A:TRP:HB3	5	0.41
(2,484)	1:4:A:CYS:H	1:5:A:VAL:H	9	0.41
(2,484)	1:4:A:CYS:H	1:5:A:VAL:H	10	0.41
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	6	0.41
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	6	0.41
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	6	0.41
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	6	0.41
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	6	0.41
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	6	0.41
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	5	0.41
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	5	0.41
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	5	0.41
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	6	0.41
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	6	0.41
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	6	0.41
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	10	0.41
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	10	0.41
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	10	0.41
(2,185)	1:20:A:GLY:HA3	1:21:A:ARG:H	8	0.41
(2,99)	1:21:A:ARG:HA	1:21:A:ARG:HB3	3	0.41
(2,99)	1:21:A:ARG:HA	1:21:A:ARG:HB3	6	0.41
(1,730)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	2	0.41
(1,711)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	0.41
(1,711)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	0.41
(1,711)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	0.41
(1,658)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	4	0.41
(1,658)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	4	0.41
(1,632)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	8	0.41
(1,632)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	9	0.41
(1,575)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,575)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	9	0.41
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	6	0.41
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	6	0.41
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	6	0.41
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	6	0.41
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	6	0.41
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	6	0.41
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.41
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.41
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.41
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	10	0.41
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	10	0.41
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	10	0.41
(1,463)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	5	0.41
(1,463)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	7	0.41
(1,450)	1:11:A:TRP:HE3	1:12:A:LEU:HG	1	0.41
(1,450)	1:11:A:TRP:HE3	1:12:A:LEU:HG	5	0.41
(1,450)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	0.41
(1,439)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	3	0.41
(1,439)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	3	0.41
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	2	0.41
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	2	0.41
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	2	0.41
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	5	0.41
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	5	0.41
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	5	0.41
(4,79)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	5	0.4
(4,64)	1:5:A:VAL:HA	1:25:A:CYS:HB3	3	0.4
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	5	0.4
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	5	0.4
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	5	0.4
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	5	0.4
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	5	0.4
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	5	0.4
(4,38)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	0.4
(4,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	0.4
(4,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	0.4
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	3	0.4
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	3	0.4
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	3	0.4
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	6	0.4
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	6	0.4
(4,13)	1:7:A:LEU:HG	1:25:A:CYS:H	1	0.4
(3,424)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	8	0.4
(3,424)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	9	0.4
(3,424)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	10	0.4
(3,58)	1:2:A:GLU:HB3	1:4:A:CYS:H	3	0.4
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	2	0.4
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	2	0.4
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	2	0.4
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	2	0.4
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	2	0.4
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	2	0.4
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	8	0.4
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	8	0.4
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	8	0.4
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	8	0.4
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	8	0.4
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	8	0.4
(2,719)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	9	0.4
(2,719)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	9	0.4
(2,685)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	7	0.4
(2,685)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	7	0.4
(2,685)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	7	0.4
(2,685)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	8	0.4
(2,685)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	8	0.4
(2,685)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	8	0.4
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	2	0.4
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	2	0.4
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	2	0.4
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD11	2	0.4
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD12	2	0.4
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD13	2	0.4
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	7	0.4
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	7	0.4
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	7	0.4
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD11	7	0.4
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD12	7	0.4
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD13	7	0.4
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	9	0.4
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	9	0.4
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	9	0.4
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD11	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD12	9	0.4
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD13	9	0.4
(2,628)	1:14:A:ASP:HB3	1:15:A:GLY:H	8	0.4
(2,618)	1:6:A:ARG:HA	1:8:A:TYR:H	2	0.4
(2,612)	1:19:A:SER:HB2	1:19:A:SER:HG	8	0.4
(2,612)	1:19:A:SER:HB2	1:19:A:SER:HG	10	0.4
(2,600)	1:11:A:TRP:H	1:11:A:TRP:HB3	9	0.4
(2,600)	1:11:A:TRP:H	1:11:A:TRP:HB3	10	0.4
(2,557)	1:23:A:PRO:HA	1:24:A:PRO:HD2	10	0.4
(2,536)	1:22:A:PRO:HB2	1:23:A:PRO:HD2	2	0.4
(2,529)	1:1:A:GLU:HA	1:1:A:GLU:HB3	7	0.4
(2,521)	1:14:A:ASP:HB2	1:16:A:GLY:H	7	0.4
(2,433)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	1	0.4
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	10	0.4
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	10	0.4
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	10	0.4
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	10	0.4
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	10	0.4
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	10	0.4
(2,402)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	7	0.4
(2,402)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	7	0.4
(2,363)	1:11:A:TRP:HZ2	1:22:A:PRO:HA	8	0.4
(2,355)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	1	0.4
(2,337)	1:22:A:PRO:HA	1:23:A:PRO:HG2	4	0.4
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	1	0.4
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	1	0.4
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	1	0.4
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	7	0.4
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	7	0.4
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	7	0.4
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	8	0.4
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	8	0.4
(2,292)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	8	0.4
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	9	0.4
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	9	0.4
(2,185)	1:20:A:GLY:HA3	1:21:A:ARG:H	4	0.4
(2,154)	1:25:A:CYS:H	1:25:A:CYS:HB2	3	0.4
(2,136)	1:18:A:SER:H	1:18:A:SER:HA	5	0.4
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG2	1	0.4
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG3	1	0.4
(2,99)	1:21:A:ARG:HA	1:21:A:ARG:HB3	1	0.4
(2,99)	1:21:A:ARG:HA	1:21:A:ARG:HB3	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:10:A:GLN:H	1:10:A:GLN:HB2	2	0.4
(2,68)	1:10:A:GLN:H	1:10:A:GLN:HB2	3	0.4
(1,749)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	5	0.4
(1,675)	1:5:A:VAL:HA	1:25:A:CYS:HB3	3	0.4
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	5	0.4
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	5	0.4
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	5	0.4
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	5	0.4
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	5	0.4
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	5	0.4
(1,463)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	8	0.4
(1,463)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	9	0.4
(1,463)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	10	0.4
(1,450)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	0.4
(1,439)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	0.4
(1,439)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	0.4
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	3	0.4
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	3	0.4
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	3	0.4
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	6	0.4
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	6	0.4
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	6	0.4
(1,252)	1:7:A:LEU:HG	1:25:A:CYS:H	1	0.4
(1,60)	1:2:A:GLU:HB3	1:4:A:CYS:H	3	0.4
(4,79)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	10	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	2	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	2	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	2	0.39
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	2	0.39
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	2	0.39
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	2	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	8	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	8	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	8	0.39
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	8	0.39
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	8	0.39
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	8	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	9	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	9	0.39
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	9	0.39
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	9	0.39
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	9	0.39
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	1	0.39
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	1	0.39
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	1	0.39
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	7	0.39
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	7	0.39
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	7	0.39
(3,519)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	5	0.39
(3,479)	1:4:A:CYS:HB2	1:25:A:CYS:HB2	6	0.39
(3,424)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	6	0.39
(3,381)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	3	0.39
(3,381)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	3	0.39
(3,381)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	9	0.39
(3,381)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	9	0.39
(3,203)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	4	0.39
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	8	0.39
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	8	0.39
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	9	0.39
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	9	0.39
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	8	0.39
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	8	0.39
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	8	0.39
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD11	8	0.39
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD12	8	0.39
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD13	8	0.39
(2,656)	1:17:A:PRO:HB2	1:18:A:SER:HB3	4	0.39
(2,654)	1:3:A:GLU:HA	1:6:A:ARG:HB2	10	0.39
(2,649)	1:5:A:VAL:HA	1:25:A:CYS:HB3	1	0.39
(2,618)	1:6:A:ARG:HA	1:8:A:TYR:H	4	0.39
(2,557)	1:23:A:PRO:HA	1:24:A:PRO:HD2	3	0.39
(2,557)	1:23:A:PRO:HA	1:24:A:PRO:HD2	5	0.39
(2,557)	1:23:A:PRO:HA	1:24:A:PRO:HD2	7	0.39
(2,557)	1:23:A:PRO:HA	1:24:A:PRO:HD2	9	0.39
(2,527)	1:1:A:GLU:HA	1:1:A:GLU:HG2	2	0.39
(2,527)	1:1:A:GLU:HA	1:1:A:GLU:HG3	2	0.39
(2,495)	1:5:A:VAL:HG11	1:6:A:ARG:HA	4	0.39
(2,495)	1:5:A:VAL:HG12	1:6:A:ARG:HA	4	0.39
(2,495)	1:5:A:VAL:HG13	1:6:A:ARG:HA	4	0.39
(2,457)	1:11:A:TRP:HH2	1:17:A:PRO:HB3	5	0.39
(2,433)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	3	0.39
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	9	0.39
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	9	0.39
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	9	0.39
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	9	0.39
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	9	0.39
(2,355)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	2	0.39
(2,355)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	3	0.39
(2,355)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	4	0.39
(2,355)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	5	0.39
(2,355)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	8	0.39
(2,355)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	9	0.39
(2,355)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	10	0.39
(2,215)	1:21:A:ARG:HA	1:22:A:PRO:HD3	9	0.39
(2,193)	1:11:A:TRP:HE1	1:22:A:PRO:HA	10	0.39
(2,145)	1:10:A:GLN:HA	1:10:A:GLN:HG2	9	0.39
(2,136)	1:18:A:SER:H	1:18:A:SER:HA	2	0.39
(2,136)	1:18:A:SER:H	1:18:A:SER:HA	3	0.39
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	7	0.39
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	7	0.39
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG2	2	0.39
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG3	2	0.39
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG2	5	0.39
(2,43)	1:13:A:LYS:HA	1:13:A:LYS:HG3	5	0.39
(1,749)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	10	0.39
(1,575)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	5	0.39
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	2	0.39
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	2	0.39
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	2	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	2	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	2	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	2	0.39
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	8	0.39
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	8	0.39
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	8	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	8	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	8	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	8	0.39
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	9	0.39
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	9	0.39
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	9	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	9	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	9	0.39
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,526)	1:4:A:CYS:HB2	1:25:A:CYS:HB2	6	0.39
(1,463)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	6	0.39
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	1	0.39
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	1	0.39
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	1	0.39
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	7	0.39
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	7	0.39
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	7	0.39
(1,410)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	3	0.39
(1,410)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	3	0.39
(1,410)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	9	0.39
(1,410)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	9	0.39
(1,213)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	4	0.39
(4,79)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	6	0.38
(4,79)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	9	0.38
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	1	0.38
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	1	0.38
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	1	0.38
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	1	0.38
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	1	0.38
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	1	0.38
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG21	3	0.38
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG22	3	0.38
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG23	3	0.38
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG21	10	0.38
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG22	10	0.38
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG23	10	0.38
(4,38)	1:11:A:TRP:HE3	1:12:A:LEU:HG	2	0.38
(4,38)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	0.38
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	8	0.38
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	8	0.38
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	8	0.38
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	6	0.38
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	6	0.38
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	6	0.38
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	6	0.38
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	6	0.38
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	6	0.38
(4,3)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.38
(3,383)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	2	0.38
(3,383)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	2	0.38
(3,381)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,381)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	5	0.38
(2,741)	1:2:A:GLU:HA	1:5:A:VAL:H	6	0.38
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	4	0.38
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	4	0.38
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	10	0.38
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	10	0.38
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	7	0.38
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	7	0.38
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	7	0.38
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	7	0.38
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	7	0.38
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	7	0.38
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	7	0.38
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	7	0.38
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	7	0.38
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	7	0.38
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	7	0.38
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	7	0.38
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	9	0.38
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	9	0.38
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	9	0.38
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	9	0.38
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	9	0.38
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	9	0.38
(2,671)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	5	0.38
(2,671)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	5	0.38
(2,671)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	5	0.38
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	3	0.38
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	3	0.38
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	3	0.38
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD11	3	0.38
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD12	3	0.38
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD13	3	0.38
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	10	0.38
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	10	0.38
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	10	0.38
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD11	10	0.38
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD12	10	0.38
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD13	10	0.38
(2,612)	1:19:A:SER:HB2	1:19:A:SER:HG	3	0.38
(2,612)	1:19:A:SER:HB2	1:19:A:SER:HG	4	0.38
(2,600)	1:11:A:TRP:H	1:11:A:TRP:HB3	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,600)	1:11:A:TRP:H	1:11:A:TRP:HB3	7	0.38
(2,600)	1:11:A:TRP:H	1:11:A:TRP:HB3	8	0.38
(2,557)	1:23:A:PRO:HA	1:24:A:PRO:HD2	6	0.38
(2,527)	1:1:A:GLU:HA	1:1:A:GLU:HG2	1	0.38
(2,527)	1:1:A:GLU:HA	1:1:A:GLU:HG3	1	0.38
(2,504)	1:14:A:ASP:HB3	1:19:A:SER:HB2	8	0.38
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB2	6	0.38
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB3	6	0.38
(2,467)	1:18:A:SER:HA	1:20:A:GLY:H	7	0.38
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	1	0.38
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	1	0.38
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	1	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	1	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	1	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	1	0.38
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	3	0.38
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	3	0.38
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	3	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	3	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	3	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	3	0.38
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	7	0.38
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	7	0.38
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	7	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	7	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	7	0.38
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	7	0.38
(2,355)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	6	0.38
(2,355)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	7	0.38
(2,350)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	8	0.38
(2,278)	1:7:A:LEU:HA	1:7:A:LEU:HB3	7	0.38
(2,246)	1:7:A:LEU:HG	1:25:A:CYS:H	9	0.38
(2,183)	1:19:A:SER:H	1:19:A:SER:HG	5	0.38
(2,136)	1:18:A:SER:H	1:18:A:SER:HA	1	0.38
(2,125)	1:9:A:ILE:HA	1:9:A:ILE:HG12	9	0.38
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	8	0.38
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	8	0.38
(2,106)	1:21:A:ARG:H	1:21:A:ARG:HB2	8	0.38
(1,749)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	6	0.38
(1,749)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	9	0.38
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	1	0.38
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	1	0.38
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	1	0.38
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	1	0.38
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	1	0.38
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG21	3	0.38
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG22	3	0.38
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG23	3	0.38
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG21	10	0.38
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG22	10	0.38
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG23	10	0.38
(1,450)	1:11:A:TRP:HE3	1:12:A:LEU:HG	2	0.38
(1,450)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	0.38
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	8	0.38
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	8	0.38
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	8	0.38
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	6	0.38
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	6	0.38
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	6	0.38
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	6	0.38
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	6	0.38
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	6	0.38
(1,413)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	2	0.38
(1,413)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	2	0.38
(1,410)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	5	0.38
(1,410)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	5	0.38
(1,75)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.38
(4,79)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	3	0.37
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	7	0.37
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	7	0.37
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	7	0.37
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	7	0.37
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	7	0.37
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	7	0.37
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG21	6	0.37
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG22	6	0.37
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG23	6	0.37
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	4	0.37
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	4	0.37
(4,35)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	4	0.37
(4,15)	1:12:A:LEU:H	1:13:A:LYS:HA	4	0.37
(3,563)	1:24:A:PRO:HG2	1:25:A:CYS:H	2	0.37
(3,519)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,424)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	4	0.37
(3,383)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	5	0.37
(3,383)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	5	0.37
(3,381)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	2	0.37
(3,381)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	2	0.37
(3,381)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	10	0.37
(3,381)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	10	0.37
(2,719)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	2	0.37
(2,719)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	2	0.37
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	1	0.37
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	1	0.37
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	1	0.37
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	1	0.37
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	1	0.37
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	1	0.37
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	5	0.37
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	5	0.37
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	5	0.37
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	7	0.37
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	7	0.37
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	7	0.37
(2,678)	1:12:A:LEU:HB2	1:13:A:LYS:HD2	6	0.37
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	6	0.37
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	6	0.37
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	6	0.37
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD11	6	0.37
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD12	6	0.37
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD13	6	0.37
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	7	0.37
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	7	0.37
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	7	0.37
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	7	0.37
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	7	0.37
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	7	0.37
(2,612)	1:19:A:SER:HB2	1:19:A:SER:HG	1	0.37
(2,612)	1:19:A:SER:HB2	1:19:A:SER:HG	2	0.37
(2,612)	1:19:A:SER:HB2	1:19:A:SER:HG	5	0.37
(2,600)	1:11:A:TRP:H	1:11:A:TRP:HB3	1	0.37
(2,557)	1:23:A:PRO:HA	1:24:A:PRO:HD2	2	0.37
(2,529)	1:1:A:GLU:HA	1:1:A:GLU:HB3	6	0.37
(2,524)	1:4:A:CYS:HA	1:7:A:LEU:HB3	1	0.37
(2,504)	1:14:A:ASP:HB3	1:19:A:SER:HB2	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,465)	1:10:A:GLN:HA	1:10:A:GLN:HE22	5	0.37
(2,445)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	1	0.37
(2,445)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	1	0.37
(2,445)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	5	0.37
(2,445)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	5	0.37
(2,350)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	1	0.37
(2,350)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	7	0.37
(2,319)	1:23:A:PRO:HA	1:23:A:PRO:HB3	1	0.37
(2,319)	1:23:A:PRO:HA	1:23:A:PRO:HB3	7	0.37
(2,319)	1:23:A:PRO:HA	1:23:A:PRO:HB3	8	0.37
(2,278)	1:7:A:LEU:HA	1:7:A:LEU:HB3	8	0.37
(2,245)	1:24:A:PRO:HB2	1:25:A:CYS:H	10	0.37
(2,229)	1:10:A:GLN:HB3	1:11:A:TRP:H	1	0.37
(2,183)	1:19:A:SER:H	1:19:A:SER:HG	1	0.37
(2,133)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	1	0.37
(2,133)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	2	0.37
(2,133)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	3	0.37
(2,133)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	4	0.37
(2,133)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	5	0.37
(2,133)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	6	0.37
(2,133)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	8	0.37
(2,133)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	9	0.37
(2,133)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	10	0.37
(2,125)	1:9:A:ILE:HA	1:9:A:ILE:HG12	2	0.37
(2,125)	1:9:A:ILE:HA	1:9:A:ILE:HG12	5	0.37
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	6	0.37
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	6	0.37
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG2	3	0.37
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG3	3	0.37
(1,749)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	3	0.37
(1,622)	1:24:A:PRO:HG2	1:25:A:CYS:H	2	0.37
(1,575)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	1	0.37
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	7	0.37
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	7	0.37
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	7	0.37
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	7	0.37
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	7	0.37
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	7	0.37
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG21	6	0.37
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG22	6	0.37
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG23	6	0.37
(1,463)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	4	0.37
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	4	0.37
(1,436)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	4	0.37
(1,413)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	5	0.37
(1,413)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	5	0.37
(1,410)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	2	0.37
(1,410)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	2	0.37
(1,410)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	10	0.37
(1,410)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	10	0.37
(1,271)	1:12:A:LEU:H	1:13:A:LYS:HA	4	0.37
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG21	2	0.36
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG22	2	0.36
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG23	2	0.36
(4,15)	1:12:A:LEU:H	1:13:A:LYS:HA	3	0.36
(4,15)	1:12:A:LEU:H	1:13:A:LYS:HA	8	0.36
(4,15)	1:12:A:LEU:H	1:13:A:LYS:HA	9	0.36
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.36
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.36
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.36
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.36
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.36
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.36
(3,657)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	1	0.36
(3,657)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	5	0.36
(3,572)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.36
(3,519)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	8	0.36
(3,424)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	3	0.36
(2,741)	1:2:A:GLU:HA	1:5:A:VAL:H	8	0.36
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	3	0.36
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	3	0.36
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	3	0.36
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	3	0.36
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	3	0.36
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	3	0.36
(2,719)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	10	0.36
(2,719)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	10	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	2	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	2	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	2	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	8	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	8	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	9	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	9	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	9	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	10	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	10	0.36
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	10	0.36
(2,678)	1:12:A:LEU:HB2	1:13:A:LYS:HD2	5	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD11	2	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD12	2	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD13	2	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD21	2	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD22	2	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD23	2	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD11	5	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD12	5	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD13	5	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD21	5	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD22	5	0.36
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD23	5	0.36
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	5	0.36
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	5	0.36
(2,667)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	5	0.36
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD11	5	0.36
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD12	5	0.36
(2,667)	1:8:A:TYR:HB3	1:12:A:LEU:HD13	5	0.36
(2,628)	1:14:A:ASP:HB3	1:15:A:GLY:H	6	0.36
(2,557)	1:23:A:PRO:HA	1:24:A:PRO:HD2	4	0.36
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB2	4	0.36
(2,503)	1:5:A:VAL:HA	1:8:A:TYR:HB3	4	0.36
(2,433)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	2	0.36
(2,393)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	7	0.36
(2,376)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	2	0.36
(2,350)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	2	0.36
(2,350)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	4	0.36
(2,350)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	5	0.36
(2,350)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	9	0.36
(2,350)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.36
(2,319)	1:23:A:PRO:HA	1:23:A:PRO:HB3	2	0.36
(2,319)	1:23:A:PRO:HA	1:23:A:PRO:HB3	3	0.36
(2,319)	1:23:A:PRO:HA	1:23:A:PRO:HB3	4	0.36
(2,319)	1:23:A:PRO:HA	1:23:A:PRO:HB3	5	0.36
(2,319)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,317)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	2	0.36
(2,317)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	3	0.36
(2,317)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	6	0.36
(2,317)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	8	0.36
(2,268)	1:11:A:TRP:H	1:12:A:LEU:HA	7	0.36
(2,200)	1:22:A:PRO:HA	1:22:A:PRO:HB3	4	0.36
(2,136)	1:18:A:SER:H	1:18:A:SER:HA	4	0.36
(2,136)	1:18:A:SER:H	1:18:A:SER:HA	6	0.36
(2,133)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	7	0.36
(2,125)	1:9:A:ILE:HA	1:9:A:ILE:HG12	3	0.36
(2,125)	1:9:A:ILE:HA	1:9:A:ILE:HG12	7	0.36
(2,125)	1:9:A:ILE:HA	1:9:A:ILE:HG12	8	0.36
(2,125)	1:9:A:ILE:HA	1:9:A:ILE:HG12	10	0.36
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	1	0.36
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	1	0.36
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	2	0.36
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	2	0.36
(2,95)	1:2:A:GLU:HG2	1:5:A:VAL:H	5	0.36
(2,36)	1:12:A:LEU:HB2	1:13:A:LYS:H	10	0.36
(1,730)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	1	0.36
(1,730)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	5	0.36
(1,631)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.36
(1,575)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	8	0.36
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG21	2	0.36
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG22	2	0.36
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG23	2	0.36
(1,463)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	3	0.36
(1,271)	1:12:A:LEU:H	1:13:A:LYS:HA	3	0.36
(1,271)	1:12:A:LEU:H	1:13:A:LYS:HA	8	0.36
(1,271)	1:12:A:LEU:H	1:13:A:LYS:HA	9	0.36
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.36
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.36
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.36
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.36
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.36
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.36
(4,79)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	8	0.35
(4,64)	1:5:A:VAL:HA	1:25:A:CYS:HB3	2	0.35
(4,57)	1:8:A:TYR:H	1:9:A:ILE:HB	1	0.35
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	1	0.35
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	1	0.35
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	1	0.35
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	1	0.35
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	1	0.35
(4,15)	1:12:A:LEU:H	1:13:A:LYS:HA	7	0.35
(4,3)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.35
(3,657)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	4	0.35
(3,563)	1:24:A:PRO:HG2	1:25:A:CYS:H	4	0.35
(3,563)	1:24:A:PRO:HG2	1:25:A:CYS:H	5	0.35
(3,519)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	7	0.35
(3,430)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	4	0.35
(3,430)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	8	0.35
(3,430)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	10	0.35
(3,424)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	1	0.35
(3,381)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	8	0.35
(3,381)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	8	0.35
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	10	0.35
(2,726)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	10	0.35
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	10	0.35
(2,726)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	10	0.35
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	10	0.35
(2,726)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	10	0.35
(2,719)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	3	0.35
(2,719)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	3	0.35
(2,719)	1:3:A:GLU:HB2	1:4:A:CYS:HB3	5	0.35
(2,719)	1:3:A:GLU:HB3	1:4:A:CYS:HB3	5	0.35
(2,717)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	1	0.35
(2,678)	1:12:A:LEU:HB2	1:13:A:LYS:HD2	9	0.35
(2,600)	1:11:A:TRP:H	1:11:A:TRP:HB3	3	0.35
(2,566)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	6	0.35
(2,557)	1:23:A:PRO:HA	1:24:A:PRO:HD2	1	0.35
(2,543)	1:6:A:ARG:HA	1:9:A:ILE:HG21	1	0.35
(2,543)	1:6:A:ARG:HA	1:9:A:ILE:HG22	1	0.35
(2,543)	1:6:A:ARG:HA	1:9:A:ILE:HG23	1	0.35
(2,510)	1:8:A:TYR:HA	1:24:A:PRO:HD2	4	0.35
(2,480)	1:19:A:SER:H	1:20:A:GLY:H	6	0.35
(2,438)	1:8:A:TYR:HE1	1:23:A:PRO:HG3	2	0.35
(2,438)	1:8:A:TYR:HE2	1:23:A:PRO:HG3	2	0.35
(2,438)	1:8:A:TYR:HE1	1:23:A:PRO:HG3	8	0.35
(2,438)	1:8:A:TYR:HE2	1:23:A:PRO:HG3	8	0.35
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG21	1	0.35
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG22	1	0.35
(2,416)	1:8:A:TYR:HE1	1:9:A:ILE:HG23	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG21	1	0.35
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG22	1	0.35
(2,416)	1:8:A:TYR:HE2	1:9:A:ILE:HG23	1	0.35
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	7	0.35
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	7	0.35
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	7	0.35
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	7	0.35
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	7	0.35
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	7	0.35
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	8	0.35
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	8	0.35
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	8	0.35
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	8	0.35
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	8	0.35
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	8	0.35
(2,402)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	8	0.35
(2,402)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	8	0.35
(2,393)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	1	0.35
(2,363)	1:11:A:TRP:HZ2	1:22:A:PRO:HA	3	0.35
(2,363)	1:11:A:TRP:HZ2	1:22:A:PRO:HA	9	0.35
(2,363)	1:11:A:TRP:HZ2	1:22:A:PRO:HA	10	0.35
(2,350)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	3	0.35
(2,350)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	6	0.35
(2,319)	1:23:A:PRO:HA	1:23:A:PRO:HB3	6	0.35
(2,319)	1:23:A:PRO:HA	1:23:A:PRO:HB3	9	0.35
(2,317)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	1	0.35
(2,317)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	5	0.35
(2,317)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	7	0.35
(2,317)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	9	0.35
(2,317)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.35
(2,278)	1:7:A:LEU:HA	1:7:A:LEU:HB3	3	0.35
(2,278)	1:7:A:LEU:HA	1:7:A:LEU:HB3	4	0.35
(2,278)	1:7:A:LEU:HA	1:7:A:LEU:HB3	9	0.35
(2,245)	1:24:A:PRO:HB2	1:25:A:CYS:H	6	0.35
(2,244)	1:2:A:GLU:HB2	1:5:A:VAL:H	2	0.35
(2,229)	1:10:A:GLN:HB3	1:11:A:TRP:H	2	0.35
(2,184)	1:19:A:SER:HG	1:21:A:ARG:H	7	0.35
(2,154)	1:25:A:CYS:H	1:25:A:CYS:HB2	8	0.35
(2,136)	1:18:A:SER:H	1:18:A:SER:HA	9	0.35
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	10	0.35
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	10	0.35
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG2	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG3	7	0.35
(2,36)	1:12:A:LEU:HB2	1:13:A:LYS:H	6	0.35
(1,749)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	8	0.35
(1,730)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	4	0.35
(1,675)	1:5:A:VAL:HA	1:25:A:CYS:HB3	2	0.35
(1,622)	1:24:A:PRO:HG2	1:25:A:CYS:H	4	0.35
(1,622)	1:24:A:PRO:HG2	1:25:A:CYS:H	5	0.35
(1,605)	1:8:A:TYR:H	1:9:A:ILE:HB	1	0.35
(1,575)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	7	0.35
(1,469)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	4	0.35
(1,469)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	8	0.35
(1,469)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	10	0.35
(1,463)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	1	0.35
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	1	0.35
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	1	0.35
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	1	0.35
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	1	0.35
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	1	0.35
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	1	0.35
(1,410)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	8	0.35
(1,410)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	8	0.35
(1,271)	1:12:A:LEU:H	1:13:A:LYS:HA	7	0.35
(1,75)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.35
(4,79)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	7	0.34
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	8	0.34
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	8	0.34
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	8	0.34
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	8	0.34
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	8	0.34
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	8	0.34
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	10	0.34
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	10	0.34
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	10	0.34
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	10	0.34
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	10	0.34
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	10	0.34
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	4	0.34
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	4	0.34
(4,54)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	4	0.34
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	4	0.34
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	4	0.34
(4,54)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG21	5	0.34
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG22	5	0.34
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG23	5	0.34
(4,15)	1:12:A:LEU:H	1:13:A:LYS:HA	2	0.34
(4,15)	1:12:A:LEU:H	1:13:A:LYS:HA	5	0.34
(4,3)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.34
(4,3)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.34
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.34
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.34
(3,657)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	10	0.34
(3,573)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	6	0.34
(3,563)	1:24:A:PRO:HG2	1:25:A:CYS:H	3	0.34
(3,519)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	2	0.34
(3,430)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	9	0.34
(3,424)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	2	0.34
(3,423)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	1	0.34
(3,423)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	1	0.34
(3,423)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	7	0.34
(3,423)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	7	0.34
(3,381)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,381)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	7	0.34
(2,685)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	9	0.34
(2,685)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	9	0.34
(2,685)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	9	0.34
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	3	0.34
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	3	0.34
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	3	0.34
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	8	0.34
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	8	0.34
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	8	0.34
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	8	0.34
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	8	0.34
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	8	0.34
(2,625)	1:19:A:SER:HG	1:20:A:GLY:H	4	0.34
(2,625)	1:19:A:SER:HG	1:20:A:GLY:H	9	0.34
(2,618)	1:6:A:ARG:HA	1:8:A:TYR:H	6	0.34
(2,600)	1:11:A:TRP:H	1:11:A:TRP:HB3	4	0.34
(2,566)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	2	0.34
(2,566)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.34
(2,529)	1:1:A:GLU:HA	1:1:A:GLU:HB3	2	0.34
(2,529)	1:1:A:GLU:HA	1:1:A:GLU:HB3	10	0.34
(2,512)	1:23:A:PRO:HD3	1:24:A:PRO:HD2	4	0.34
(2,467)	1:18:A:SER:HA	1:20:A:GLY:H	10	0.34
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	2	0.34
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	2	0.34
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	2	0.34
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	2	0.34
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	2	0.34
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	2	0.34
(2,393)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.34
(2,363)	1:11:A:TRP:HZ2	1:22:A:PRO:HA	5	0.34
(2,317)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	4	0.34
(2,278)	1:7:A:LEU:HA	1:7:A:LEU:HB3	2	0.34
(2,278)	1:7:A:LEU:HA	1:7:A:LEU:HB3	5	0.34
(2,278)	1:7:A:LEU:HA	1:7:A:LEU:HB3	10	0.34
(2,193)	1:11:A:TRP:HE1	1:22:A:PRO:HA	7	0.34
(2,193)	1:11:A:TRP:HE1	1:22:A:PRO:HA	8	0.34
(2,154)	1:25:A:CYS:H	1:25:A:CYS:HB2	7	0.34
(2,154)	1:25:A:CYS:H	1:25:A:CYS:HB2	9	0.34
(2,120)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	2	0.34
(2,111)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	6	0.34
(2,109)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	9	0.34
(2,106)	1:21:A:ARG:H	1:21:A:ARG:HB2	10	0.34
(2,61)	1:4:A:CYS:H	1:4:A:CYS:HB3	7	0.34
(2,49)	1:13:A:LYS:HA	1:13:A:LYS:HE2	2	0.34
(2,36)	1:12:A:LEU:HB2	1:13:A:LYS:H	2	0.34
(2,36)	1:12:A:LEU:HB2	1:13:A:LYS:H	7	0.34
(1,749)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	7	0.34
(1,730)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	10	0.34
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	8	0.34
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	8	0.34
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	8	0.34
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	8	0.34
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	8	0.34
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	8	0.34
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	10	0.34
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	10	0.34
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	10	0.34
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	10	0.34
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	10	0.34
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	10	0.34
(1,632)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	6	0.34
(1,622)	1:24:A:PRO:HG2	1:25:A:CYS:H	3	0.34
(1,575)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	2	0.34
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	4	0.34
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	4	0.34
(1,569)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	4	0.34
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD21	4	0.34
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD22	4	0.34
(1,569)	1:8:A:TYR:HB3	1:12:A:LEU:HD23	4	0.34
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG21	5	0.34
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG22	5	0.34
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG23	5	0.34
(1,469)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	9	0.34
(1,463)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	2	0.34
(1,462)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	1	0.34
(1,462)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	1	0.34
(1,462)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	7	0.34
(1,462)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	7	0.34
(1,410)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	7	0.34
(1,410)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	7	0.34
(1,271)	1:12:A:LEU:H	1:13:A:LYS:HA	2	0.34
(1,271)	1:12:A:LEU:H	1:13:A:LYS:HA	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.34
(1,75)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.34
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.34
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.34
(4,76)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	5	0.33
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	3	0.33
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	3	0.33
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	3	0.33
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	3	0.33
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	3	0.33
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	3	0.33
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG21	4	0.33
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG22	4	0.33
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG23	4	0.33
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG21	9	0.33
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG22	9	0.33
(4,53)	1:6:A:ARG:HA	1:9:A:ILE:HG23	9	0.33
(4,15)	1:12:A:LEU:H	1:13:A:LYS:HA	1	0.33
(4,15)	1:12:A:LEU:H	1:13:A:LYS:HA	6	0.33
(4,3)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,3)	1:6:A:ARG:H	1:6:A:ARG:HB3	7	0.33
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.33
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.33
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.33
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.33
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.33
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.33
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.33
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.33
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.33
(3,657)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	7	0.33
(3,573)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	7	0.33
(3,563)	1:24:A:PRO:HG2	1:25:A:CYS:H	7	0.33
(3,563)	1:24:A:PRO:HG2	1:25:A:CYS:H	8	0.33
(3,563)	1:24:A:PRO:HG2	1:25:A:CYS:H	9	0.33
(3,563)	1:24:A:PRO:HG2	1:25:A:CYS:H	10	0.33
(3,491)	1:10:A:GLN:HG3	1:11:A:TRP:H	10	0.33
(3,184)	1:18:A:SER:H	1:19:A:SER:HB2	8	0.33
(3,50)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	5	0.33
(3,50)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	5	0.33
(2,678)	1:12:A:LEU:HB2	1:13:A:LYS:HD2	7	0.33
(2,648)	1:11:A:TRP:HA	1:21:A:ARG:HD2	2	0.33
(2,600)	1:11:A:TRP:H	1:11:A:TRP:HB3	2	0.33
(2,566)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	5	0.33
(2,566)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	7	0.33
(2,480)	1:19:A:SER:H	1:20:A:GLY:H	10	0.33
(2,438)	1:8:A:TYR:HE1	1:23:A:PRO:HG3	1	0.33
(2,438)	1:8:A:TYR:HE2	1:23:A:PRO:HG3	1	0.33
(2,426)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	1	0.33
(2,426)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	1	0.33
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	4	0.33
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	4	0.33
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	4	0.33
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	4	0.33
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	4	0.33
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	6	0.33
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	6	0.33
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	6	0.33
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	6	0.33
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	6	0.33
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	6	0.33
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	10	0.33
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	10	0.33
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	10	0.33
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	10	0.33
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	10	0.33
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	10	0.33
(2,402)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	4	0.33
(2,402)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	4	0.33
(2,393)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	8	0.33
(2,363)	1:11:A:TRP:HZ2	1:22:A:PRO:HA	7	0.33
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	1	0.33
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	1	0.33
(2,193)	1:11:A:TRP:HE1	1:22:A:PRO:HA	9	0.33
(2,183)	1:19:A:SER:H	1:19:A:SER:HG	2	0.33
(2,183)	1:19:A:SER:H	1:19:A:SER:HG	3	0.33
(2,183)	1:19:A:SER:H	1:19:A:SER:HG	7	0.33
(2,146)	1:10:A:GLN:HA	1:10:A:GLN:HG3	7	0.33
(2,145)	1:10:A:GLN:HA	1:10:A:GLN:HG2	8	0.33
(2,136)	1:18:A:SER:H	1:18:A:SER:HA	8	0.33
(2,120)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	1	0.33
(2,120)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	3	0.33
(2,120)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	4	0.33
(2,120)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	5	0.33
(2,120)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	6	0.33
(2,120)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	7	0.33
(2,120)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	8	0.33
(2,120)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	9	0.33
(2,108)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	4	0.33
(2,102)	1:21:A:ARG:H	1:21:A:ARG:HD2	6	0.33
(2,99)	1:21:A:ARG:HA	1:21:A:ARG:HB3	4	0.33
(2,61)	1:4:A:CYS:H	1:4:A:CYS:HB3	8	0.33
(2,36)	1:12:A:LEU:HB2	1:13:A:LYS:H	8	0.33
(1,743)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,730)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	7	0.33
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	3	0.33
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	3	0.33
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	3	0.33
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	3	0.33
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	3	0.33
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	3	0.33
(1,632)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	7	0.33
(1,622)	1:24:A:PRO:HG2	1:25:A:CYS:H	7	0.33
(1,622)	1:24:A:PRO:HG2	1:25:A:CYS:H	8	0.33
(1,622)	1:24:A:PRO:HG2	1:25:A:CYS:H	9	0.33
(1,622)	1:24:A:PRO:HG2	1:25:A:CYS:H	10	0.33
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG21	4	0.33
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG22	4	0.33
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG23	4	0.33
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG21	9	0.33
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG22	9	0.33
(1,564)	1:6:A:ARG:HA	1:9:A:ILE:HG23	9	0.33
(1,540)	1:10:A:GLN:HG3	1:11:A:TRP:H	10	0.33
(1,271)	1:12:A:LEU:H	1:13:A:LYS:HA	1	0.33
(1,271)	1:12:A:LEU:H	1:13:A:LYS:HA	6	0.33
(1,193)	1:18:A:SER:H	1:19:A:SER:HB2	8	0.33
(1,75)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.33
(1,75)	1:6:A:ARG:H	1:6:A:ARG:HB3	7	0.33
(1,52)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	5	0.33
(1,52)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	5	0.33
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.33
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.33
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.33
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.33
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.33
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.33
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.33
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.33
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.33
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.33
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.33
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.33
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.33
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.33
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.33
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.33
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.33
(4,76)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	2	0.32
(4,76)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	3	0.32
(4,76)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	7	0.32
(4,66)	1:6:A:ARG:HA	1:9:A:ILE:HG13	7	0.32
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	9	0.32
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	9	0.32
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	9	0.32
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	9	0.32
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	9	0.32
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	9	0.32
(4,57)	1:8:A:TYR:H	1:9:A:ILE:HB	4	0.32
(4,57)	1:8:A:TYR:H	1:9:A:ILE:HB	9	0.32
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	7	0.32
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	7	0.32
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	7	0.32
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	7	0.32
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	7	0.32
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	7	0.32
(4,17)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	4	0.32
(4,15)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.32
(4,3)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.32
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.32
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.32
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.32
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.32
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.32
(4,2)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.32
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.32
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.32
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.32
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.32
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.32
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.32
(3,657)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	3	0.32
(3,657)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	9	0.32
(3,474)	1:4:A:CYS:HA	1:25:A:CYS:HB3	1	0.32
(3,423)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	3	0.32
(3,423)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	3	0.32
(3,423)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	9	0.32
(3,423)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,411)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	8	0.32
(3,58)	1:2:A:GLU:HB3	1:4:A:CYS:H	5	0.32
(2,737)	1:12:A:LEU:HB3	1:14:A:ASP:H	3	0.32
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH21	5	0.32
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH22	5	0.32
(2,685)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	5	0.32
(2,685)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	5	0.32
(2,685)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	5	0.32
(2,683)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	1	0.32
(2,683)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	1	0.32
(2,683)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	1	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD11	3	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD12	3	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD13	3	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD21	3	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD22	3	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD23	3	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD11	9	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD12	9	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD13	9	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD21	9	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD22	9	0.32
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD23	9	0.32
(2,648)	1:11:A:TRP:HA	1:21:A:ARG:HD2	1	0.32
(2,566)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	1	0.32
(2,566)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	3	0.32
(2,529)	1:1:A:GLU:HA	1:1:A:GLU:HB3	8	0.32
(2,511)	1:14:A:ASP:HB2	1:19:A:SER:HB2	4	0.32
(2,484)	1:4:A:CYS:H	1:5:A:VAL:H	4	0.32
(2,438)	1:8:A:TYR:HE1	1:23:A:PRO:HG3	7	0.32
(2,438)	1:8:A:TYR:HE2	1:23:A:PRO:HG3	7	0.32
(2,426)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	4	0.32
(2,426)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	4	0.32
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	3	0.32
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	3	0.32
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	3	0.32
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	3	0.32
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	3	0.32
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	3	0.32
(2,393)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	3	0.32
(2,393)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	5	0.32
(2,393)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	9	0.32
(2,376)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	5	0.32
(2,363)	1:11:A:TRP:HZ2	1:22:A:PRO:HA	6	0.32
(2,246)	1:7:A:LEU:HG	1:25:A:CYS:H	6	0.32
(2,136)	1:18:A:SER:H	1:18:A:SER:HA	10	0.32
(2,134)	1:18:A:SER:H	1:18:A:SER:HB2	10	0.32
(2,125)	1:9:A:ILE:HA	1:9:A:ILE:HG12	4	0.32
(2,125)	1:9:A:ILE:HA	1:9:A:ILE:HG12	6	0.32
(2,120)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.32
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG2	6	0.32
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG3	6	0.32
(2,95)	1:2:A:GLU:HG2	1:5:A:VAL:H	9	0.32
(2,36)	1:12:A:LEU:HB2	1:13:A:LYS:H	4	0.32
(2,36)	1:12:A:LEU:HB2	1:13:A:LYS:H	5	0.32
(1,743)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	2	0.32
(1,743)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	3	0.32
(1,743)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	7	0.32
(1,730)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	3	0.32
(1,730)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	9	0.32
(1,681)	1:6:A:ARG:HA	1:9:A:ILE:HG13	7	0.32
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	9	0.32
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	9	0.32
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	9	0.32
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	9	0.32
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	9	0.32
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	9	0.32
(1,605)	1:8:A:TYR:H	1:9:A:ILE:HB	4	0.32
(1,605)	1:8:A:TYR:H	1:9:A:ILE:HB	9	0.32
(1,521)	1:4:A:CYS:HA	1:25:A:CYS:HB3	1	0.32
(1,462)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	3	0.32
(1,462)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	3	0.32
(1,462)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	9	0.32
(1,462)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	9	0.32
(1,448)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	8	0.32
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	7	0.32
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	7	0.32
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	7	0.32
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	7	0.32
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	7	0.32
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	7	0.32
(1,278)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	4	0.32
(1,271)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.32
(1,60)	1:2:A:GLU:HB3	1:4:A:CYS:H	5	0.32
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.32
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.32
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.32
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.32
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.32
(1,22)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.32
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.32
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.32
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.32
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.32
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.32
(1,6)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.32
(4,76)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	9	0.31
(4,66)	1:6:A:ARG:HA	1:9:A:ILE:HG13	8	0.31
(4,57)	1:8:A:TYR:H	1:9:A:ILE:HB	3	0.31
(4,57)	1:8:A:TYR:H	1:9:A:ILE:HB	6	0.31
(4,57)	1:8:A:TYR:H	1:9:A:ILE:HB	10	0.31
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.31
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.31
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.31
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.31
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.31
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.31
(4,17)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	2	0.31
(4,17)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	3	0.31
(4,17)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	8	0.31
(4,14)	1:10:A:GLN:HA	1:11:A:TRP:H	1	0.31
(4,14)	1:10:A:GLN:HA	1:11:A:TRP:H	2	0.31
(3,563)	1:24:A:PRO:HG2	1:25:A:CYS:H	6	0.31
(3,519)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	4	0.31
(3,423)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	6	0.31
(3,423)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	6	0.31
(3,423)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	10	0.31
(3,423)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	10	0.31
(3,383)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	8	0.31
(3,383)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	8	0.31
(3,50)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	7	0.31
(3,50)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	7	0.31
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	3	0.31
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,722)	1:5:A:VAL:HB	1:9:A:ILE:HG12	1	0.31
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	9	0.31
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	9	0.31
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	9	0.31
(2,678)	1:12:A:LEU:HB2	1:13:A:LYS:HD2	4	0.31
(2,648)	1:11:A:TRP:HA	1:21:A:ARG:HD2	6	0.31
(2,625)	1:19:A:SER:HG	1:20:A:GLY:H	7	0.31
(2,608)	1:6:A:ARG:HA	1:9:A:ILE:HB	9	0.31
(2,566)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	4	0.31
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	1	0.31
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	1	0.31
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	2	0.31
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	2	0.31
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	5	0.31
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	5	0.31
(2,529)	1:1:A:GLU:HA	1:1:A:GLU:HB3	1	0.31
(2,426)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	6	0.31
(2,426)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	6	0.31
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	5	0.31
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	5	0.31
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	5	0.31
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	5	0.31
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	5	0.31
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	5	0.31
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	9	0.31
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	9	0.31
(2,412)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	9	0.31
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	9	0.31
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	9	0.31
(2,412)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	9	0.31
(2,393)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	2	0.31
(2,363)	1:11:A:TRP:HZ2	1:22:A:PRO:HA	2	0.31
(2,320)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	1	0.31
(2,320)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	2	0.31
(2,320)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	3	0.31
(2,320)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	4	0.31
(2,320)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	5	0.31
(2,320)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	6	0.31
(2,320)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	7	0.31
(2,320)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	8	0.31
(2,320)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	9	0.31
(2,320)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,268)	1:11:A:TRP:H	1:12:A:LEU:HA	6	0.31
(2,242)	1:17:A:PRO:HB2	1:18:A:SER:H	8	0.31
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	10	0.31
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	10	0.31
(2,166)	1:19:A:SER:H	1:19:A:SER:HB3	6	0.31
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG2	5	0.31
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG3	5	0.31
(2,71)	1:5:A:VAL:H	1:5:A:VAL:HB	4	0.31
(2,36)	1:12:A:LEU:HB2	1:13:A:LYS:H	3	0.31
(1,743)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	9	0.31
(1,681)	1:6:A:ARG:HA	1:9:A:ILE:HG13	8	0.31
(1,622)	1:24:A:PRO:HG2	1:25:A:CYS:H	6	0.31
(1,605)	1:8:A:TYR:H	1:9:A:ILE:HB	3	0.31
(1,605)	1:8:A:TYR:H	1:9:A:ILE:HB	6	0.31
(1,605)	1:8:A:TYR:H	1:9:A:ILE:HB	10	0.31
(1,575)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	4	0.31
(1,462)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	6	0.31
(1,462)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	6	0.31
(1,462)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	10	0.31
(1,462)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	10	0.31
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.31
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.31
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.31
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.31
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.31
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.31
(1,413)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	8	0.31
(1,413)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	8	0.31
(1,278)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	2	0.31
(1,278)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	3	0.31
(1,278)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	8	0.31
(1,262)	1:10:A:GLN:HA	1:11:A:TRP:H	1	0.31
(1,262)	1:10:A:GLN:HA	1:11:A:TRP:H	2	0.31
(1,52)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	7	0.31
(1,52)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	7	0.31
(4,76)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	8	0.3
(4,76)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	10	0.3
(4,63)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	0.3
(4,57)	1:8:A:TYR:H	1:9:A:ILE:HB	5	0.3
(4,57)	1:8:A:TYR:H	1:9:A:ILE:HB	8	0.3
(4,46)	1:5:A:VAL:HG21	1:6:A:ARG:HA	6	0.3
(4,46)	1:5:A:VAL:HG22	1:6:A:ARG:HA	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,46)	1:5:A:VAL:HG23	1:6:A:ARG:HA	6	0.3
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.3
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.3
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.3
(4,17)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	1	0.3
(4,17)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	5	0.3
(4,17)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	6	0.3
(4,17)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	7	0.3
(4,3)	1:6:A:ARG:H	1:6:A:ARG:HB3	2	0.3
(3,657)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	8	0.3
(3,635)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	1	0.3
(3,529)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	10	0.3
(3,58)	1:2:A:GLU:HB3	1:4:A:CYS:H	10	0.3
(3,50)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	1	0.3
(3,50)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	1	0.3
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	5	0.3
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	5	0.3
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	5	0.3
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	5	0.3
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	5	0.3
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	5	0.3
(2,680)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	2	0.3
(2,680)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	2	0.3
(2,680)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	2	0.3
(2,671)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	10	0.3
(2,671)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	10	0.3
(2,671)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	10	0.3
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	1	0.3
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	1	0.3
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	1	0.3
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	4	0.3
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	4	0.3
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	4	0.3
(2,654)	1:3:A:GLU:HA	1:6:A:ARG:HB2	2	0.3
(2,608)	1:6:A:ARG:HA	1:9:A:ILE:HB	4	0.3
(2,608)	1:6:A:ARG:HA	1:9:A:ILE:HB	5	0.3
(2,598)	1:21:A:ARG:HB2	1:21:A:ARG:HE	6	0.3
(2,566)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	8	0.3
(2,566)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	9	0.3
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	4	0.3
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	4	0.3
(2,460)	1:24:A:PRO:HD2	1:25:A:CYS:H	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,445)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	2	0.3
(2,445)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	2	0.3
(2,445)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	6	0.3
(2,445)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	6	0.3
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	2	0.3
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	2	0.3
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	2	0.3
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	2	0.3
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	2	0.3
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	2	0.3
(2,353)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	2	0.3
(2,353)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	3	0.3
(2,353)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	5	0.3
(2,353)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	8	0.3
(2,353)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	9	0.3
(2,353)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.3
(2,278)	1:7:A:LEU:HA	1:7:A:LEU:HB3	6	0.3
(2,268)	1:11:A:TRP:H	1:12:A:LEU:HA	8	0.3
(2,222)	1:8:A:TYR:H	1:9:A:ILE:H	1	0.3
(2,222)	1:8:A:TYR:H	1:9:A:ILE:H	10	0.3
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	9	0.3
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	9	0.3
(2,102)	1:21:A:ARG:H	1:21:A:ARG:HD2	1	0.3
(2,36)	1:12:A:LEU:HB2	1:13:A:LYS:H	1	0.3
(2,36)	1:12:A:LEU:HB2	1:13:A:LYS:H	9	0.3
(1,743)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	8	0.3
(1,743)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	10	0.3
(1,730)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	8	0.3
(1,702)	1:7:A:LEU:HB2	1:24:A:PRO:HG2	1	0.3
(1,663)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	0.3
(1,605)	1:8:A:TYR:H	1:9:A:ILE:HB	5	0.3
(1,605)	1:8:A:TYR:H	1:9:A:ILE:HB	8	0.3
(1,585)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	10	0.3
(1,515)	1:5:A:VAL:HG21	1:6:A:ARG:HA	6	0.3
(1,515)	1:5:A:VAL:HG22	1:6:A:ARG:HA	6	0.3
(1,515)	1:5:A:VAL:HG23	1:6:A:ARG:HA	6	0.3
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.3
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.3
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.3
(1,278)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	1	0.3
(1,278)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	5	0.3
(1,278)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,278)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	7	0.3
(1,75)	1:6:A:ARG:H	1:6:A:ARG:HB3	2	0.3
(1,60)	1:2:A:GLU:HB3	1:4:A:CYS:H	10	0.3
(1,52)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	1	0.3
(1,52)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	1	0.3
(4,75)	1:10:A:GLN:HA	1:13:A:LYS:HD2	10	0.29
(4,66)	1:6:A:ARG:HA	1:9:A:ILE:HG13	1	0.29
(4,46)	1:5:A:VAL:HG21	1:6:A:ARG:HA	4	0.29
(4,46)	1:5:A:VAL:HG22	1:6:A:ARG:HA	4	0.29
(4,46)	1:5:A:VAL:HG23	1:6:A:ARG:HA	4	0.29
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	3	0.29
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	3	0.29
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	3	0.29
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	3	0.29
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	3	0.29
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	3	0.29
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	9	0.29
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	9	0.29
(4,34)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	9	0.29
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	9	0.29
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	9	0.29
(4,34)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	9	0.29
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	8	0.29
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	8	0.29
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	8	0.29
(4,17)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	9	0.29
(4,14)	1:10:A:GLN:HA	1:11:A:TRP:H	3	0.29
(3,657)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	6	0.29
(3,50)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	3	0.29
(3,50)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	3	0.29
(3,50)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	8	0.29
(3,50)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	8	0.29
(2,737)	1:12:A:LEU:HB3	1:14:A:ASP:H	4	0.29
(2,737)	1:12:A:LEU:HB3	1:14:A:ASP:H	7	0.29
(2,737)	1:12:A:LEU:HB3	1:14:A:ASP:H	9	0.29
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	1	0.29
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	1	0.29
(2,678)	1:12:A:LEU:HB2	1:13:A:LYS:HD2	10	0.29
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	2	0.29
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	2	0.29
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	2	0.29
(2,598)	1:21:A:ARG:HB2	1:21:A:ARG:HE	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,529)	1:1:A:GLU:HA	1:1:A:GLU:HB3	3	0.29
(2,511)	1:14:A:ASP:HB2	1:19:A:SER:HB2	8	0.29
(2,484)	1:4:A:CYS:H	1:5:A:VAL:H	6	0.29
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	2	0.29
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	2	0.29
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	2	0.29
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	2	0.29
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	2	0.29
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	2	0.29
(2,402)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	2	0.29
(2,402)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	2	0.29
(2,376)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	1	0.29
(2,353)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	4	0.29
(2,353)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	6	0.29
(2,307)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	7	0.29
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.29
(2,204)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	3	0.29
(2,204)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	9	0.29
(2,200)	1:22:A:PRO:HA	1:22:A:PRO:HB3	1	0.29
(2,200)	1:22:A:PRO:HA	1:22:A:PRO:HB3	2	0.29
(2,200)	1:22:A:PRO:HA	1:22:A:PRO:HB3	3	0.29
(2,200)	1:22:A:PRO:HA	1:22:A:PRO:HB3	5	0.29
(2,200)	1:22:A:PRO:HA	1:22:A:PRO:HB3	6	0.29
(2,200)	1:22:A:PRO:HA	1:22:A:PRO:HB3	7	0.29
(2,200)	1:22:A:PRO:HA	1:22:A:PRO:HB3	9	0.29
(2,193)	1:11:A:TRP:HE1	1:22:A:PRO:HA	5	0.29
(2,185)	1:20:A:GLY:HA3	1:21:A:ARG:H	10	0.29
(2,154)	1:25:A:CYS:H	1:25:A:CYS:HB2	10	0.29
(2,139)	1:18:A:SER:HB2	1:18:A:SER:HB3	1	0.29
(2,139)	1:18:A:SER:HB2	1:18:A:SER:HB3	3	0.29
(2,139)	1:18:A:SER:HB2	1:18:A:SER:HB3	4	0.29
(2,139)	1:18:A:SER:HB2	1:18:A:SER:HB3	6	0.29
(2,139)	1:18:A:SER:HB2	1:18:A:SER:HB3	7	0.29
(2,139)	1:18:A:SER:HB2	1:18:A:SER:HB3	8	0.29
(2,139)	1:18:A:SER:HB2	1:18:A:SER:HB3	9	0.29
(2,139)	1:18:A:SER:HB2	1:18:A:SER:HB3	10	0.29
(2,95)	1:2:A:GLU:HG2	1:5:A:VAL:H	10	0.29
(2,73)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	0.29
(1,738)	1:10:A:GLN:HA	1:13:A:LYS:HD2	10	0.29
(1,730)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	6	0.29
(1,681)	1:6:A:ARG:HA	1:9:A:ILE:HG13	1	0.29
(1,515)	1:5:A:VAL:HG21	1:6:A:ARG:HA	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:5:A:VAL:HG22	1:6:A:ARG:HA	4	0.29
(1,515)	1:5:A:VAL:HG23	1:6:A:ARG:HA	4	0.29
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	3	0.29
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	3	0.29
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	3	0.29
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	3	0.29
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	3	0.29
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	3	0.29
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	9	0.29
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	9	0.29
(1,431)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	9	0.29
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	9	0.29
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	9	0.29
(1,431)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	9	0.29
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	8	0.29
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	8	0.29
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	8	0.29
(1,278)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	9	0.29
(1,262)	1:10:A:GLN:HA	1:11:A:TRP:H	3	0.29
(1,52)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	3	0.29
(1,52)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	3	0.29
(1,52)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	8	0.29
(1,52)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	8	0.29
(4,75)	1:10:A:GLN:HA	1:13:A:LYS:HD2	6	0.28
(4,64)	1:5:A:VAL:HA	1:25:A:CYS:HB3	7	0.28
(4,57)	1:8:A:TYR:H	1:9:A:ILE:HB	2	0.28
(4,57)	1:8:A:TYR:H	1:9:A:ILE:HB	7	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	1	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	1	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	1	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	2	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	2	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	2	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	3	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	3	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	3	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	5	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	5	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	5	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	7	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	7	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	9	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	9	0.28
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	9	0.28
(4,17)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	10	0.28
(4,14)	1:10:A:GLN:HA	1:11:A:TRP:H	4	0.28
(4,14)	1:10:A:GLN:HA	1:11:A:TRP:H	7	0.28
(3,653)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	3	0.28
(3,653)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	3	0.28
(3,653)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	3	0.28
(3,653)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	3	0.28
(3,653)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	3	0.28
(3,653)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	3	0.28
(3,529)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	2	0.28
(3,529)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	5	0.28
(3,529)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	6	0.28
(3,58)	1:2:A:GLU:HB3	1:4:A:CYS:H	7	0.28
(3,50)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	9	0.28
(3,50)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	9	0.28
(2,685)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	3	0.28
(2,685)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	3	0.28
(2,685)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	3	0.28
(2,685)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.28
(2,685)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.28
(2,685)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.28
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	8	0.28
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	8	0.28
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	8	0.28
(2,522)	1:3:A:GLU:HG2	1:4:A:CYS:HA	5	0.28
(2,522)	1:3:A:GLU:HG3	1:4:A:CYS:HA	5	0.28
(2,522)	1:3:A:GLU:HG2	1:4:A:CYS:HA	7	0.28
(2,522)	1:3:A:GLU:HG3	1:4:A:CYS:HA	7	0.28
(2,515)	1:2:A:GLU:HA	1:2:A:GLU:HB2	4	0.28
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	5	0.28
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	5	0.28
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	5	0.28
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	5	0.28
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	5	0.28
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	5	0.28
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	5	0.28
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	5	0.28
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	5	0.28
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	5	0.28
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	5	0.28
(2,402)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	3	0.28
(2,402)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	3	0.28
(2,376)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	7	0.28
(2,376)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	8	0.28
(2,353)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	1	0.28
(2,353)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	7	0.28
(2,328)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	8	0.28
(2,286)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	4	0.28
(2,286)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	6	0.28
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	8	0.28
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	8	0.28
(2,222)	1:8:A:TYR:H	1:9:A:ILE:H	5	0.28
(2,222)	1:8:A:TYR:H	1:9:A:ILE:H	6	0.28
(2,222)	1:8:A:TYR:H	1:9:A:ILE:H	7	0.28
(2,204)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	1	0.28
(2,204)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	2	0.28
(2,204)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	5	0.28
(2,204)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	6	0.28
(2,204)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	7	0.28
(2,200)	1:22:A:PRO:HA	1:22:A:PRO:HB3	8	0.28
(2,200)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.28
(2,193)	1:11:A:TRP:HE1	1:22:A:PRO:HA	1	0.28
(2,145)	1:10:A:GLN:HA	1:10:A:GLN:HG2	4	0.28
(2,139)	1:18:A:SER:HB2	1:18:A:SER:HB3	2	0.28
(2,139)	1:18:A:SER:HB2	1:18:A:SER:HB3	5	0.28
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	5	0.28
(2,113)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	5	0.28
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	4	0.28
(2,112)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	4	0.28
(2,73)	1:6:A:ARG:H	1:6:A:ARG:HB2	2	0.28
(2,73)	1:6:A:ARG:H	1:6:A:ARG:HB2	6	0.28
(2,64)	1:4:A:CYS:HA	1:4:A:CYS:HB2	8	0.28
(1,738)	1:10:A:GLN:HA	1:13:A:LYS:HD2	6	0.28
(1,726)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	3	0.28
(1,726)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	3	0.28
(1,726)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	3	0.28
(1,726)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	3	0.28
(1,726)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	3	0.28
(1,726)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	3	0.28
(1,675)	1:5:A:VAL:HA	1:25:A:CYS:HB3	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:8:A:TYR:H	1:9:A:ILE:HB	2	0.28
(1,605)	1:8:A:TYR:H	1:9:A:ILE:HB	7	0.28
(1,585)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	2	0.28
(1,585)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	5	0.28
(1,585)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	6	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	1	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	1	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	1	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	2	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	2	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	2	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	3	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	3	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	3	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	5	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	5	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	5	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	7	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	7	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	7	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	9	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	9	0.28
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	9	0.28
(1,278)	1:11:A:TRP:HB2	1:11:A:TRP:HE1	10	0.28
(1,262)	1:10:A:GLN:HA	1:11:A:TRP:H	4	0.28
(1,262)	1:10:A:GLN:HA	1:11:A:TRP:H	7	0.28
(1,60)	1:2:A:GLU:HB3	1:4:A:CYS:H	7	0.28
(1,52)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	9	0.28
(1,52)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	9	0.28
(4,63)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	5	0.27
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	6	0.27
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	6	0.27
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	6	0.27
(4,9)	1:24:A:PRO:HA	1:25:A:CYS:H	1	0.27
(4,3)	1:6:A:ARG:H	1:6:A:ARG:HB3	1	0.27
(3,653)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	9	0.27
(3,653)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	9	0.27
(3,653)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	9	0.27
(3,653)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	9	0.27
(3,653)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	9	0.27
(3,653)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	9	0.27
(3,491)	1:10:A:GLN:HG3	1:11:A:TRP:H	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,472)	1:8:A:TYR:HA	1:11:A:TRP:HB2	4	0.27
(3,58)	1:2:A:GLU:HB3	1:4:A:CYS:H	9	0.27
(2,737)	1:12:A:LEU:HB3	1:14:A:ASP:H	8	0.27
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	4	0.27
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	4	0.27
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	4	0.27
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	6	0.27
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	6	0.27
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	6	0.27
(2,675)	1:12:A:LEU:HB3	1:13:A:LYS:HD2	2	0.27
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD11	10	0.27
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD12	10	0.27
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD13	10	0.27
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD21	10	0.27
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD22	10	0.27
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD23	10	0.27
(2,671)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	3	0.27
(2,671)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	3	0.27
(2,671)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	3	0.27
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	7	0.27
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	7	0.27
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	7	0.27
(2,582)	1:7:A:LEU:HG	1:8:A:TYR:H	7	0.27
(2,582)	1:7:A:LEU:HG	1:8:A:TYR:H	9	0.27
(2,556)	1:23:A:PRO:HA	1:24:A:PRO:HD3	8	0.27
(2,515)	1:2:A:GLU:HA	1:2:A:GLU:HB2	3	0.27
(2,508)	1:14:A:ASP:HB3	1:19:A:SER:HA	9	0.27
(2,362)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	6	0.27
(2,360)	1:11:A:TRP:HD1	1:19:A:SER:HG	7	0.27
(2,328)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	1	0.27
(2,328)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	2	0.27
(2,328)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	3	0.27
(2,328)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	5	0.27
(2,328)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	6	0.27
(2,328)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	7	0.27
(2,328)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.27
(2,307)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	1	0.27
(2,307)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	3	0.27
(2,307)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	5	0.27
(2,286)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	1	0.27
(2,286)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	2	0.27
(2,286)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,286)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	5	0.27
(2,286)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	7	0.27
(2,286)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	8	0.27
(2,286)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	9	0.27
(2,286)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	10	0.27
(2,246)	1:7:A:LEU:HG	1:25:A:CYS:H	3	0.27
(2,233)	1:9:A:ILE:H	1:9:A:ILE:HG13	1	0.27
(2,229)	1:10:A:GLN:HB3	1:11:A:TRP:H	3	0.27
(2,222)	1:8:A:TYR:H	1:9:A:ILE:H	8	0.27
(2,222)	1:8:A:TYR:H	1:9:A:ILE:H	9	0.27
(2,204)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	8	0.27
(2,204)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.27
(2,185)	1:20:A:GLY:HA3	1:21:A:ARG:H	9	0.27
(2,109)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	4	0.27
(2,102)	1:21:A:ARG:H	1:21:A:ARG:HD2	3	0.27
(2,73)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.27
(2,73)	1:6:A:ARG:H	1:6:A:ARG:HB2	4	0.27
(2,73)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.27
(2,71)	1:5:A:VAL:H	1:5:A:VAL:HB	6	0.27
(1,726)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	9	0.27
(1,726)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	9	0.27
(1,726)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	9	0.27
(1,726)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	9	0.27
(1,726)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	9	0.27
(1,726)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	9	0.27
(1,663)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	5	0.27
(1,540)	1:10:A:GLN:HG3	1:11:A:TRP:H	9	0.27
(1,519)	1:8:A:TYR:HA	1:11:A:TRP:HB2	4	0.27
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	6	0.27
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	6	0.27
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	6	0.27
(1,192)	1:24:A:PRO:HA	1:25:A:CYS:H	1	0.27
(1,75)	1:6:A:ARG:H	1:6:A:ARG:HB3	1	0.27
(1,60)	1:2:A:GLU:HB3	1:4:A:CYS:H	9	0.27
(4,68)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	4	0.26
(4,68)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	4	0.26
(4,68)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	4	0.26
(4,66)	1:6:A:ARG:HA	1:9:A:ILE:HG13	4	0.26
(4,66)	1:6:A:ARG:HA	1:9:A:ILE:HG13	6	0.26
(4,63)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	6	0.26
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	1	0.26
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	1	0.26
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	1	0.26
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	1	0.26
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	1	0.26
(4,45)	1:4:A:CYS:HA	1:7:A:LEU:HB2	6	0.26
(4,37)	1:23:A:PRO:HB2	1:25:A:CYS:H	8	0.26
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	4	0.26
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	4	0.26
(4,20)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	4	0.26
(4,9)	1:24:A:PRO:HA	1:25:A:CYS:H	7	0.26
(3,529)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	3	0.26
(3,381)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	1	0.26
(3,381)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	1	0.26
(3,50)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	4	0.26
(3,50)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	4	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	3	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	3	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	3	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	6	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	6	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	6	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	9	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	9	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	9	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	10	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	10	0.26
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	10	0.26
(2,608)	1:6:A:ARG:HA	1:9:A:ILE:HB	3	0.26
(2,608)	1:6:A:ARG:HA	1:9:A:ILE:HB	10	0.26
(2,556)	1:23:A:PRO:HA	1:24:A:PRO:HD3	7	0.26
(2,445)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	4	0.26
(2,445)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	4	0.26
(2,426)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	3	0.26
(2,426)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	3	0.26
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	9	0.26
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	9	0.26
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	9	0.26
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	9	0.26
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	9	0.26
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	9	0.26
(2,394)	1:8:A:TYR:HE1	1:24:A:PRO:HD2	8	0.26
(2,394)	1:8:A:TYR:HE2	1:24:A:PRO:HD2	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	4	0.26
(2,360)	1:11:A:TRP:HD1	1:19:A:SER:HG	8	0.26
(2,328)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	9	0.26
(2,311)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	1	0.26
(2,311)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	2	0.26
(2,311)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	3	0.26
(2,311)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	4	0.26
(2,311)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	5	0.26
(2,311)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	6	0.26
(2,311)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	7	0.26
(2,311)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	8	0.26
(2,311)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.26
(2,268)	1:11:A:TRP:H	1:12:A:LEU:HA	5	0.26
(2,212)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	1	0.26
(2,212)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	2	0.26
(2,212)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	3	0.26
(2,212)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	4	0.26
(2,212)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	5	0.26
(2,212)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	6	0.26
(2,212)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	7	0.26
(2,212)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	8	0.26
(2,212)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	9	0.26
(2,212)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.26
(2,193)	1:11:A:TRP:HE1	1:22:A:PRO:HA	6	0.26
(2,145)	1:10:A:GLN:HA	1:10:A:GLN:HG2	10	0.26
(2,73)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.26
(2,73)	1:6:A:ARG:H	1:6:A:ARG:HB2	9	0.26
(2,73)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.26
(2,64)	1:4:A:CYS:HA	1:4:A:CYS:HB2	7	0.26
(1,711)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	4	0.26
(1,711)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	4	0.26
(1,711)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	4	0.26
(1,681)	1:6:A:ARG:HA	1:9:A:ILE:HG13	4	0.26
(1,681)	1:6:A:ARG:HA	1:9:A:ILE:HG13	6	0.26
(1,663)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	6	0.26
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	1	0.26
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	1	0.26
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	1	0.26
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	1	0.26
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	1	0.26
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	1	0.26
(1,585)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,514)	1:4:A:CYS:HA	1:7:A:LEU:HB2	6	0.26
(1,443)	1:23:A:PRO:HB2	1:25:A:CYS:H	8	0.26
(1,410)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	1	0.26
(1,410)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	1	0.26
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	4	0.26
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	4	0.26
(1,295)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	4	0.26
(1,192)	1:24:A:PRO:HA	1:25:A:CYS:H	7	0.26
(1,52)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	4	0.26
(1,52)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	4	0.26
(4,64)	1:5:A:VAL:HA	1:25:A:CYS:HB3	8	0.25
(4,63)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	9	0.25
(4,62)	1:6:A:ARG:HB2	1:7:A:LEU:H	4	0.25
(4,14)	1:10:A:GLN:HA	1:11:A:TRP:H	5	0.25
(4,14)	1:10:A:GLN:HA	1:11:A:TRP:H	6	0.25
(4,14)	1:10:A:GLN:HA	1:11:A:TRP:H	8	0.25
(4,9)	1:24:A:PRO:HA	1:25:A:CYS:H	8	0.25
(4,9)	1:24:A:PRO:HA	1:25:A:CYS:H	9	0.25
(4,9)	1:24:A:PRO:HA	1:25:A:CYS:H	10	0.25
(3,653)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	10	0.25
(3,653)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	10	0.25
(3,653)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	10	0.25
(3,653)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	10	0.25
(3,653)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	10	0.25
(3,653)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	10	0.25
(3,610)	1:11:A:TRP:HA	1:21:A:ARG:HD3	4	0.25
(3,529)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	7	0.25
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH21	9	0.25
(2,733)	1:14:A:ASP:HB2	1:21:A:ARG:HH22	9	0.25
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB2	3	0.25
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB2	3	0.25
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB2	3	0.25
(2,696)	1:9:A:ILE:HG21	1:13:A:LYS:HB3	3	0.25
(2,696)	1:9:A:ILE:HG22	1:13:A:LYS:HB3	3	0.25
(2,696)	1:9:A:ILE:HG23	1:13:A:LYS:HB3	3	0.25
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD21	5	0.25
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD22	5	0.25
(2,666)	1:11:A:TRP:HB2	1:12:A:LEU:HD23	5	0.25
(2,610)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.25
(2,582)	1:7:A:LEU:HG	1:8:A:TYR:H	5	0.25
(2,522)	1:3:A:GLU:HG2	1:4:A:CYS:HA	2	0.25
(2,522)	1:3:A:GLU:HG3	1:4:A:CYS:HA	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,516)	1:2:A:GLU:HA	1:2:A:GLU:HB3	5	0.25
(2,516)	1:2:A:GLU:HA	1:2:A:GLU:HB3	10	0.25
(2,477)	1:18:A:SER:H	1:19:A:SER:H	6	0.25
(2,426)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	7	0.25
(2,426)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	7	0.25
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	8	0.25
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	8	0.25
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	8	0.25
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	8	0.25
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	8	0.25
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	8	0.25
(2,399)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	9	0.25
(2,328)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	4	0.25
(2,313)	1:19:A:SER:HB2	1:19:A:SER:HB3	6	0.25
(2,311)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	9	0.25
(2,246)	1:7:A:LEU:HG	1:25:A:CYS:H	5	0.25
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB2	4	0.25
(2,241)	1:10:A:GLN:HE21	1:13:A:LYS:HB3	4	0.25
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.25
(2,222)	1:8:A:TYR:H	1:9:A:ILE:H	2	0.25
(2,222)	1:8:A:TYR:H	1:9:A:ILE:H	3	0.25
(2,222)	1:8:A:TYR:H	1:9:A:ILE:H	4	0.25
(2,182)	1:18:A:SER:HA	1:19:A:SER:H	3	0.25
(2,152)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	4	0.25
(2,152)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	10	0.25
(2,102)	1:21:A:ARG:H	1:21:A:ARG:HD2	4	0.25
(2,73)	1:6:A:ARG:H	1:6:A:ARG:HB2	8	0.25
(2,24)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	4	0.25
(2,24)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	6	0.25
(2,24)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	7	0.25
(2,24)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	8	0.25
(2,24)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	9	0.25
(2,8)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	4	0.25
(2,8)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	6	0.25
(2,8)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	7	0.25
(2,8)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	8	0.25
(2,8)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	9	0.25
(1,726)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	10	0.25
(1,726)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	10	0.25
(1,726)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	10	0.25
(1,726)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	10	0.25
(1,726)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,726)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	10	0.25
(1,675)	1:5:A:VAL:HA	1:25:A:CYS:HB3	8	0.25
(1,673)	1:11:A:TRP:HA	1:21:A:ARG:HD3	4	0.25
(1,663)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	9	0.25
(1,643)	1:6:A:ARG:HB2	1:7:A:LEU:H	4	0.25
(1,585)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	7	0.25
(1,262)	1:10:A:GLN:HA	1:11:A:TRP:H	5	0.25
(1,262)	1:10:A:GLN:HA	1:11:A:TRP:H	6	0.25
(1,262)	1:10:A:GLN:HA	1:11:A:TRP:H	8	0.25
(1,192)	1:24:A:PRO:HA	1:25:A:CYS:H	8	0.25
(1,192)	1:24:A:PRO:HA	1:25:A:CYS:H	9	0.25
(1,192)	1:24:A:PRO:HA	1:25:A:CYS:H	10	0.25
(4,76)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	4	0.24
(4,75)	1:10:A:GLN:HA	1:13:A:LYS:HD2	2	0.24
(4,66)	1:6:A:ARG:HA	1:9:A:ILE:HG13	3	0.24
(4,66)	1:6:A:ARG:HA	1:9:A:ILE:HG13	9	0.24
(4,63)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	2	0.24
(4,63)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	3	0.24
(4,63)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	8	0.24
(4,37)	1:23:A:PRO:HB2	1:25:A:CYS:H	7	0.24
(4,9)	1:24:A:PRO:HA	1:25:A:CYS:H	2	0.24
(4,9)	1:24:A:PRO:HA	1:25:A:CYS:H	3	0.24
(4,9)	1:24:A:PRO:HA	1:25:A:CYS:H	5	0.24
(4,9)	1:24:A:PRO:HA	1:25:A:CYS:H	6	0.24
(3,655)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	8	0.24
(3,573)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	5	0.24
(3,529)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	4	0.24
(3,107)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	6	0.24
(2,741)	1:2:A:GLU:HA	1:5:A:VAL:H	1	0.24
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	5	0.24
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	5	0.24
(2,713)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	8	0.24
(2,713)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	8	0.24
(2,671)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	4	0.24
(2,671)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	4	0.24
(2,671)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	4	0.24
(2,671)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	8	0.24
(2,671)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	8	0.24
(2,671)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	8	0.24
(2,625)	1:19:A:SER:HG	1:20:A:GLY:H	8	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB2	1	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB3	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB2	2	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB3	2	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB2	3	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB3	3	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB2	5	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB3	5	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB2	6	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB3	6	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB2	9	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB3	9	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB2	10	0.24
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB3	10	0.24
(2,582)	1:7:A:LEU:HG	1:8:A:TYR:H	8	0.24
(2,569)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	8	0.24
(2,556)	1:23:A:PRO:HA	1:24:A:PRO:HD3	1	0.24
(2,549)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	8	0.24
(2,549)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	8	0.24
(2,549)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	8	0.24
(2,549)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	8	0.24
(2,549)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	8	0.24
(2,549)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	8	0.24
(2,516)	1:2:A:GLU:HA	1:2:A:GLU:HB3	1	0.24
(2,462)	1:4:A:CYS:HB3	1:5:A:VAL:H	6	0.24
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	4	0.24
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	4	0.24
(2,420)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	4	0.24
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	4	0.24
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	4	0.24
(2,420)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	4	0.24
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	4	0.24
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	4	0.24
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	4	0.24
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	4	0.24
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	4	0.24
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	4	0.24
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	0.24
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	0.24
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	0.24
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	0.24
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	0.24
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	0.24
(2,376)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD1	1	0.24
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD2	1	0.24
(2,334)	1:22:A:PRO:HA	1:23:A:PRO:HD3	2	0.24
(2,313)	1:19:A:SER:HB2	1:19:A:SER:HB3	7	0.24
(2,313)	1:19:A:SER:HB2	1:19:A:SER:HB3	10	0.24
(2,277)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	1	0.24
(2,277)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	2	0.24
(2,277)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	3	0.24
(2,277)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	4	0.24
(2,277)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	5	0.24
(2,277)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	6	0.24
(2,277)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	7	0.24
(2,277)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	8	0.24
(2,277)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	9	0.24
(2,277)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.24
(2,244)	1:2:A:GLU:HB2	1:5:A:VAL:H	9	0.24
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HG	7	0.24
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.24
(2,204)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	4	0.24
(2,146)	1:10:A:GLN:HA	1:10:A:GLN:HG3	5	0.24
(2,146)	1:10:A:GLN:HA	1:10:A:GLN:HG3	6	0.24
(2,135)	1:18:A:SER:H	1:18:A:SER:HB3	6	0.24
(2,102)	1:21:A:ARG:H	1:21:A:ARG:HD2	2	0.24
(2,102)	1:21:A:ARG:H	1:21:A:ARG:HD2	7	0.24
(2,95)	1:2:A:GLU:HG2	1:5:A:VAL:H	3	0.24
(2,24)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	1	0.24
(2,24)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	2	0.24
(2,24)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	3	0.24
(2,24)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	5	0.24
(2,24)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.24
(2,8)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	1	0.24
(2,8)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	2	0.24
(2,8)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	3	0.24
(2,8)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	5	0.24
(2,8)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.24
(1,743)	1:24:A:PRO:HB2	1:25:A:CYS:HB3	4	0.24
(1,738)	1:10:A:GLN:HA	1:13:A:LYS:HD2	2	0.24
(1,728)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	8	0.24
(1,681)	1:6:A:ARG:HA	1:9:A:ILE:HG13	3	0.24
(1,681)	1:6:A:ARG:HA	1:9:A:ILE:HG13	9	0.24
(1,663)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	2	0.24
(1,663)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	8	0.24
(1,632)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	5	0.24
(1,585)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	4	0.24
(1,443)	1:23:A:PRO:HB2	1:25:A:CYS:H	7	0.24
(1,192)	1:24:A:PRO:HA	1:25:A:CYS:H	2	0.24
(1,192)	1:24:A:PRO:HA	1:25:A:CYS:H	3	0.24
(1,192)	1:24:A:PRO:HA	1:25:A:CYS:H	5	0.24
(1,192)	1:24:A:PRO:HA	1:25:A:CYS:H	6	0.24
(1,112)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	6	0.24
(4,75)	1:10:A:GLN:HA	1:13:A:LYS:HD2	1	0.23
(4,68)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	6	0.23
(4,68)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	6	0.23
(4,68)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	6	0.23
(4,66)	1:6:A:ARG:HA	1:9:A:ILE:HG13	2	0.23
(4,66)	1:6:A:ARG:HA	1:9:A:ILE:HG13	10	0.23
(4,62)	1:6:A:ARG:HB2	1:7:A:LEU:H	1	0.23
(3,653)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	5	0.23
(3,653)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	5	0.23
(3,653)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	5	0.23
(3,653)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	5	0.23
(3,653)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	5	0.23
(3,653)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	5	0.23
(3,529)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	9	0.23
(3,222)	1:11:A:TRP:H	1:24:A:PRO:HG2	10	0.23
(3,50)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	10	0.23
(3,50)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	10	0.23
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	2	0.23
(2,735)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	2	0.23
(2,685)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	2	0.23
(2,685)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	2	0.23
(2,685)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	2	0.23
(2,680)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	1	0.23
(2,680)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	1	0.23
(2,680)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	1	0.23
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	9	0.23
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	9	0.23
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	9	0.23
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	9	0.23
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	9	0.23
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	9	0.23
(2,610)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	0.23
(2,608)	1:6:A:ARG:HA	1:9:A:ILE:HB	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB2	4	0.23
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB3	4	0.23
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB2	7	0.23
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB3	7	0.23
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB2	8	0.23
(2,591)	1:8:A:TYR:HA	1:8:A:TYR:HB3	8	0.23
(2,582)	1:7:A:LEU:HG	1:8:A:TYR:H	2	0.23
(2,556)	1:23:A:PRO:HA	1:24:A:PRO:HD3	10	0.23
(2,516)	1:2:A:GLU:HA	1:2:A:GLU:HB3	6	0.23
(2,516)	1:2:A:GLU:HA	1:2:A:GLU:HB3	7	0.23
(2,515)	1:2:A:GLU:HA	1:2:A:GLU:HB2	2	0.23
(2,515)	1:2:A:GLU:HA	1:2:A:GLU:HB2	9	0.23
(2,457)	1:11:A:TRP:HH2	1:17:A:PRO:HB3	1	0.23
(2,457)	1:11:A:TRP:HH2	1:17:A:PRO:HB3	2	0.23
(2,376)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	3	0.23
(2,313)	1:19:A:SER:HB2	1:19:A:SER:HB3	8	0.23
(2,313)	1:19:A:SER:HB2	1:19:A:SER:HB3	9	0.23
(2,307)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	2	0.23
(2,294)	1:12:A:LEU:HD21	1:12:A:LEU:HG	3	0.23
(2,294)	1:12:A:LEU:HD22	1:12:A:LEU:HG	3	0.23
(2,294)	1:12:A:LEU:HD23	1:12:A:LEU:HG	3	0.23
(2,294)	1:12:A:LEU:HD21	1:12:A:LEU:HG	5	0.23
(2,294)	1:12:A:LEU:HD22	1:12:A:LEU:HG	5	0.23
(2,294)	1:12:A:LEU:HD23	1:12:A:LEU:HG	5	0.23
(2,294)	1:12:A:LEU:HD21	1:12:A:LEU:HG	9	0.23
(2,294)	1:12:A:LEU:HD22	1:12:A:LEU:HG	9	0.23
(2,294)	1:12:A:LEU:HD23	1:12:A:LEU:HG	9	0.23
(2,294)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.23
(2,294)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.23
(2,294)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.23
(2,244)	1:2:A:GLU:HB2	1:5:A:VAL:H	10	0.23
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HG	4	0.23
(2,193)	1:11:A:TRP:HE1	1:22:A:PRO:HA	3	0.23
(2,167)	1:19:A:SER:HA	1:19:A:SER:HB2	9	0.23
(2,167)	1:19:A:SER:HA	1:19:A:SER:HB2	10	0.23
(2,110)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	9	0.23
(2,109)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	6	0.23
(2,95)	1:2:A:GLU:HG2	1:5:A:VAL:H	2	0.23
(1,738)	1:10:A:GLN:HA	1:13:A:LYS:HD2	1	0.23
(1,726)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	5	0.23
(1,726)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	5	0.23
(1,726)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,726)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	5	0.23
(1,726)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	5	0.23
(1,726)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	5	0.23
(1,711)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	6	0.23
(1,711)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	6	0.23
(1,711)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	6	0.23
(1,681)	1:6:A:ARG:HA	1:9:A:ILE:HG13	2	0.23
(1,681)	1:6:A:ARG:HA	1:9:A:ILE:HG13	10	0.23
(1,643)	1:6:A:ARG:HB2	1:7:A:LEU:H	1	0.23
(1,585)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	9	0.23
(1,232)	1:11:A:TRP:H	1:24:A:PRO:HG2	10	0.23
(1,52)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	10	0.23
(1,52)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	10	0.23
(4,79)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	1	0.22
(4,63)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	7	0.22
(4,62)	1:6:A:ARG:HB2	1:7:A:LEU:H	7	0.22
(4,19)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.22
(4,19)	1:7:A:LEU:H	1:7:A:LEU:HB2	5	0.22
(4,19)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.22
(4,19)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.22
(4,9)	1:24:A:PRO:HA	1:25:A:CYS:H	4	0.22
(3,655)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	10	0.22
(3,653)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	2	0.22
(3,653)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	2	0.22
(3,653)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	2	0.22
(3,653)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	2	0.22
(3,653)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	2	0.22
(3,653)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	2	0.22
(3,620)	1:7:A:LEU:HD11	1:25:A:CYS:HA	6	0.22
(3,620)	1:7:A:LEU:HD12	1:25:A:CYS:HA	6	0.22
(3,620)	1:7:A:LEU:HD13	1:25:A:CYS:HA	6	0.22
(3,620)	1:7:A:LEU:HD21	1:25:A:CYS:HA	6	0.22
(3,620)	1:7:A:LEU:HD22	1:25:A:CYS:HA	6	0.22
(3,620)	1:7:A:LEU:HD23	1:25:A:CYS:HA	6	0.22
(3,573)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	4	0.22
(3,563)	1:24:A:PRO:HG2	1:25:A:CYS:H	1	0.22
(3,529)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	1	0.22
(3,529)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	8	0.22
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	7	0.22
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	7	0.22
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	7	0.22
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	8	0.22
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	8	0.22
(3,334)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	1	0.22
(2,720)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	4	0.22
(2,713)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	7	0.22
(2,713)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	7	0.22
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	1	0.22
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	1	0.22
(2,684)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	1	0.22
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	1	0.22
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	1	0.22
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	1	0.22
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	1	0.22
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	1	0.22
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	1	0.22
(2,608)	1:6:A:ARG:HA	1:9:A:ILE:HB	6	0.22
(2,569)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	9	0.22
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	6	0.22
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	6	0.22
(2,552)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	6	0.22
(2,524)	1:4:A:CYS:HA	1:7:A:LEU:HB3	6	0.22
(2,516)	1:2:A:GLU:HA	1:2:A:GLU:HB3	3	0.22
(2,516)	1:2:A:GLU:HA	1:2:A:GLU:HB3	8	0.22
(2,515)	1:2:A:GLU:HA	1:2:A:GLU:HB2	5	0.22
(2,515)	1:2:A:GLU:HA	1:2:A:GLU:HB2	6	0.22
(2,494)	1:5:A:VAL:HG21	1:6:A:ARG:HA	7	0.22
(2,494)	1:5:A:VAL:HG22	1:6:A:ARG:HA	7	0.22
(2,494)	1:5:A:VAL:HG23	1:6:A:ARG:HA	7	0.22
(2,477)	1:18:A:SER:H	1:19:A:SER:H	9	0.22
(2,452)	1:11:A:TRP:HE3	1:23:A:PRO:HA	10	0.22
(2,438)	1:8:A:TYR:HE1	1:23:A:PRO:HG3	5	0.22
(2,438)	1:8:A:TYR:HE2	1:23:A:PRO:HG3	5	0.22
(2,425)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	1	0.22
(2,425)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	1	0.22
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	6	0.22
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	6	0.22
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	6	0.22
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	6	0.22
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	6	0.22
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	6	0.22
(2,394)	1:8:A:TYR:HE1	1:24:A:PRO:HD2	5	0.22
(2,394)	1:8:A:TYR:HE2	1:24:A:PRO:HD2	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,376)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	9	0.22
(2,313)	1:19:A:SER:HB2	1:19:A:SER:HB3	1	0.22
(2,313)	1:19:A:SER:HB2	1:19:A:SER:HB3	2	0.22
(2,313)	1:19:A:SER:HB2	1:19:A:SER:HB3	3	0.22
(2,313)	1:19:A:SER:HB2	1:19:A:SER:HB3	4	0.22
(2,313)	1:19:A:SER:HB2	1:19:A:SER:HB3	5	0.22
(2,294)	1:12:A:LEU:HD21	1:12:A:LEU:HG	1	0.22
(2,294)	1:12:A:LEU:HD22	1:12:A:LEU:HG	1	0.22
(2,294)	1:12:A:LEU:HD23	1:12:A:LEU:HG	1	0.22
(2,294)	1:12:A:LEU:HD21	1:12:A:LEU:HG	2	0.22
(2,294)	1:12:A:LEU:HD22	1:12:A:LEU:HG	2	0.22
(2,294)	1:12:A:LEU:HD23	1:12:A:LEU:HG	2	0.22
(2,294)	1:12:A:LEU:HD21	1:12:A:LEU:HG	4	0.22
(2,294)	1:12:A:LEU:HD22	1:12:A:LEU:HG	4	0.22
(2,294)	1:12:A:LEU:HD23	1:12:A:LEU:HG	4	0.22
(2,294)	1:12:A:LEU:HD21	1:12:A:LEU:HG	6	0.22
(2,294)	1:12:A:LEU:HD22	1:12:A:LEU:HG	6	0.22
(2,294)	1:12:A:LEU:HD23	1:12:A:LEU:HG	6	0.22
(2,294)	1:12:A:LEU:HD21	1:12:A:LEU:HG	7	0.22
(2,294)	1:12:A:LEU:HD22	1:12:A:LEU:HG	7	0.22
(2,294)	1:12:A:LEU:HD23	1:12:A:LEU:HG	7	0.22
(2,294)	1:12:A:LEU:HD21	1:12:A:LEU:HG	8	0.22
(2,294)	1:12:A:LEU:HD22	1:12:A:LEU:HG	8	0.22
(2,294)	1:12:A:LEU:HD23	1:12:A:LEU:HG	8	0.22
(2,268)	1:11:A:TRP:H	1:12:A:LEU:HA	9	0.22
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.22
(2,207)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	9	0.22
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG21	1	0.22
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG22	1	0.22
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG23	1	0.22
(2,152)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	8	0.22
(2,137)	1:18:A:SER:HA	1:18:A:SER:HB3	6	0.22
(2,125)	1:9:A:ILE:HA	1:9:A:ILE:HG12	1	0.22
(2,109)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	10	0.22
(2,88)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	10	0.22
(1,749)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	1	0.22
(1,728)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	10	0.22
(1,726)	1:7:A:LEU:HD11	1:24:A:PRO:HG3	2	0.22
(1,726)	1:7:A:LEU:HD12	1:24:A:PRO:HG3	2	0.22
(1,726)	1:7:A:LEU:HD13	1:24:A:PRO:HG3	2	0.22
(1,726)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	2	0.22
(1,726)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,726)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	2	0.22
(1,686)	1:7:A:LEU:HD11	1:25:A:CYS:HA	6	0.22
(1,686)	1:7:A:LEU:HD12	1:25:A:CYS:HA	6	0.22
(1,686)	1:7:A:LEU:HD13	1:25:A:CYS:HA	6	0.22
(1,686)	1:7:A:LEU:HD21	1:25:A:CYS:HA	6	0.22
(1,686)	1:7:A:LEU:HD22	1:25:A:CYS:HA	6	0.22
(1,686)	1:7:A:LEU:HD23	1:25:A:CYS:HA	6	0.22
(1,663)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	7	0.22
(1,643)	1:6:A:ARG:HB2	1:7:A:LEU:H	7	0.22
(1,632)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	4	0.22
(1,622)	1:24:A:PRO:HG2	1:25:A:CYS:H	1	0.22
(1,585)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	1	0.22
(1,585)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	8	0.22
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	7	0.22
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	7	0.22
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	7	0.22
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	8	0.22
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	8	0.22
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	8	0.22
(1,357)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	1	0.22
(1,291)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.22
(1,291)	1:7:A:LEU:H	1:7:A:LEU:HB2	5	0.22
(1,291)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.22
(1,291)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.22
(1,192)	1:24:A:PRO:HA	1:25:A:CYS:H	4	0.22
(4,66)	1:6:A:ARG:HA	1:9:A:ILE:HG13	5	0.21
(4,62)	1:6:A:ARG:HB2	1:7:A:LEU:H	2	0.21
(4,62)	1:6:A:ARG:HB2	1:7:A:LEU:H	3	0.21
(4,62)	1:6:A:ARG:HB2	1:7:A:LEU:H	9	0.21
(4,45)	1:4:A:CYS:HA	1:7:A:LEU:HB2	4	0.21
(4,41)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	8	0.21
(4,41)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.21
(4,19)	1:7:A:LEU:H	1:7:A:LEU:HB2	2	0.21
(4,19)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.21
(4,19)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.21
(4,19)	1:7:A:LEU:H	1:7:A:LEU:HB2	7	0.21
(4,19)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.21
(4,14)	1:10:A:GLN:HA	1:11:A:TRP:H	9	0.21
(4,7)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	7	0.21
(4,5)	1:14:A:ASP:H	1:14:A:ASP:HB3	5	0.21
(4,5)	1:14:A:ASP:H	1:14:A:ASP:HB3	8	0.21
(3,647)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,647)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	7	0.21
(3,647)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	7	0.21
(3,513)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	2	0.21
(3,491)	1:10:A:GLN:HG3	1:11:A:TRP:H	8	0.21
(3,472)	1:8:A:TYR:HA	1:11:A:TRP:HB2	2	0.21
(3,472)	1:8:A:TYR:HA	1:11:A:TRP:HB2	6	0.21
(3,334)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	2	0.21
(3,334)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	3	0.21
(3,334)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	4	0.21
(3,334)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	5	0.21
(3,334)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	9	0.21
(3,68)	1:10:A:GLN:H	1:10:A:GLN:HB3	8	0.21
(3,68)	1:10:A:GLN:H	1:10:A:GLN:HB3	10	0.21
(2,737)	1:12:A:LEU:HB3	1:14:A:ASP:H	5	0.21
(2,644)	1:8:A:TYR:HE1	1:11:A:TRP:HZ3	9	0.21
(2,644)	1:8:A:TYR:HE2	1:11:A:TRP:HZ3	9	0.21
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	3	0.21
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	3	0.21
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	3	0.21
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	3	0.21
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	3	0.21
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	3	0.21
(2,582)	1:7:A:LEU:HG	1:8:A:TYR:H	3	0.21
(2,582)	1:7:A:LEU:HG	1:8:A:TYR:H	10	0.21
(2,576)	1:6:A:ARG:H	1:8:A:TYR:H	8	0.21
(2,569)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	1	0.21
(2,556)	1:23:A:PRO:HA	1:24:A:PRO:HD3	9	0.21
(2,549)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	7	0.21
(2,549)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	7	0.21
(2,549)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	7	0.21
(2,549)	1:5:A:VAL:HG11	1:8:A:TYR:HB3	7	0.21
(2,549)	1:5:A:VAL:HG12	1:8:A:TYR:HB3	7	0.21
(2,549)	1:5:A:VAL:HG13	1:8:A:TYR:HB3	7	0.21
(2,517)	1:2:A:GLU:HA	1:3:A:GLU:H	7	0.21
(2,517)	1:2:A:GLU:HA	1:3:A:GLU:H	8	0.21
(2,516)	1:2:A:GLU:HA	1:2:A:GLU:HB3	2	0.21
(2,516)	1:2:A:GLU:HA	1:2:A:GLU:HB3	9	0.21
(2,515)	1:2:A:GLU:HA	1:2:A:GLU:HB2	10	0.21
(2,494)	1:5:A:VAL:HG21	1:6:A:ARG:HA	8	0.21
(2,494)	1:5:A:VAL:HG22	1:6:A:ARG:HA	8	0.21
(2,494)	1:5:A:VAL:HG23	1:6:A:ARG:HA	8	0.21
(2,481)	1:20:A:GLY:H	1:21:A:ARG:H	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	3	0.21
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	3	0.21
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	3	0.21
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	3	0.21
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	3	0.21
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	3	0.21
(2,399)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	10	0.21
(2,394)	1:8:A:TYR:HE1	1:24:A:PRO:HD2	2	0.21
(2,394)	1:8:A:TYR:HE2	1:24:A:PRO:HD2	2	0.21
(2,376)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	10	0.21
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD1	6	0.21
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD2	6	0.21
(2,334)	1:22:A:PRO:HA	1:23:A:PRO:HD3	6	0.21
(2,290)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	1	0.21
(2,290)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	2	0.21
(2,290)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	3	0.21
(2,290)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	5	0.21
(2,290)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	6	0.21
(2,282)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	4	0.21
(2,282)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	7	0.21
(2,282)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	8	0.21
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HG	3	0.21
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.21
(2,229)	1:10:A:GLN:HB3	1:11:A:TRP:H	4	0.21
(2,207)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	2	0.21
(2,207)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	3	0.21
(2,207)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	5	0.21
(2,207)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	6	0.21
(2,185)	1:20:A:GLY:HA3	1:21:A:ARG:H	6	0.21
(2,182)	1:18:A:SER:HA	1:19:A:SER:H	5	0.21
(2,152)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	9	0.21
(2,138)	1:18:A:SER:HA	1:18:A:SER:HB2	3	0.21
(2,138)	1:18:A:SER:HA	1:18:A:SER:HB2	4	0.21
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG21	1	0.21
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG22	1	0.21
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG23	1	0.21
(2,110)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	10	0.21
(2,88)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	1	0.21
(2,88)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	2	0.21
(2,88)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	4	0.21
(2,88)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	5	0.21
(2,88)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,88)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	7	0.21
(2,88)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	8	0.21
(2,88)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	9	0.21
(2,71)	1:5:A:VAL:H	1:5:A:VAL:HB	1	0.21
(2,49)	1:13:A:LYS:HA	1:13:A:LYS:HE2	6	0.21
(1,716)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	7	0.21
(1,716)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	7	0.21
(1,716)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	7	0.21
(1,681)	1:6:A:ARG:HA	1:9:A:ILE:HG13	5	0.21
(1,643)	1:6:A:ARG:HB2	1:7:A:LEU:H	2	0.21
(1,643)	1:6:A:ARG:HB2	1:7:A:LEU:H	3	0.21
(1,643)	1:6:A:ARG:HB2	1:7:A:LEU:H	9	0.21
(1,566)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	2	0.21
(1,540)	1:10:A:GLN:HG3	1:11:A:TRP:H	8	0.21
(1,519)	1:8:A:TYR:HA	1:11:A:TRP:HB2	2	0.21
(1,519)	1:8:A:TYR:HA	1:11:A:TRP:HB2	6	0.21
(1,514)	1:4:A:CYS:HA	1:7:A:LEU:HB2	4	0.21
(1,506)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	8	0.21
(1,506)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.21
(1,357)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	2	0.21
(1,357)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	3	0.21
(1,357)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	4	0.21
(1,357)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	5	0.21
(1,357)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	9	0.21
(1,291)	1:7:A:LEU:H	1:7:A:LEU:HB2	2	0.21
(1,291)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.21
(1,291)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.21
(1,291)	1:7:A:LEU:H	1:7:A:LEU:HB2	7	0.21
(1,291)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.21
(1,262)	1:10:A:GLN:HA	1:11:A:TRP:H	9	0.21
(1,154)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	7	0.21
(1,86)	1:14:A:ASP:H	1:14:A:ASP:HB3	5	0.21
(1,86)	1:14:A:ASP:H	1:14:A:ASP:HB3	8	0.21
(1,70)	1:10:A:GLN:H	1:10:A:GLN:HB3	8	0.21
(1,70)	1:10:A:GLN:H	1:10:A:GLN:HB3	10	0.21
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	1	0.2
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	1	0.2
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	1	0.2
(4,62)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.2
(4,41)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	1	0.2
(4,41)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	2	0.2
(4,41)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,41)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	4	0.2
(4,41)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	5	0.2
(4,41)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	6	0.2
(4,41)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	7	0.2
(4,41)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	9	0.2
(4,22)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	9	0.2
(4,7)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	1	0.2
(4,7)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	5	0.2
(4,7)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	6	0.2
(4,5)	1:14:A:ASP:H	1:14:A:ASP:HB3	6	0.2
(3,655)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	5	0.2
(3,334)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	6	0.2
(3,334)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	7	0.2
(3,334)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	8	0.2
(3,334)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.2
(3,249)	1:19:A:SER:HB2	1:21:A:ARG:H	9	0.2
(3,210)	1:21:A:ARG:HA	1:22:A:PRO:HD2	10	0.2
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	7	0.2
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	7	0.2
(2,693)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	7	0.2
(2,680)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	6	0.2
(2,680)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	6	0.2
(2,680)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	6	0.2
(2,680)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	10	0.2
(2,680)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	10	0.2
(2,680)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	10	0.2
(2,675)	1:12:A:LEU:HB3	1:13:A:LYS:HD2	1	0.2
(2,608)	1:6:A:ARG:HA	1:9:A:ILE:HB	8	0.2
(2,576)	1:6:A:ARG:H	1:8:A:TYR:H	7	0.2
(2,569)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	4	0.2
(2,517)	1:2:A:GLU:HA	1:3:A:GLU:H	2	0.2
(2,516)	1:2:A:GLU:HA	1:2:A:GLU:HB3	4	0.2
(2,515)	1:2:A:GLU:HA	1:2:A:GLU:HB2	1	0.2
(2,515)	1:2:A:GLU:HA	1:2:A:GLU:HB2	7	0.2
(2,507)	1:11:A:TRP:HA	1:14:A:ASP:HB2	7	0.2
(2,452)	1:11:A:TRP:HE3	1:23:A:PRO:HA	6	0.2
(2,438)	1:8:A:TYR:HE1	1:23:A:PRO:HG3	3	0.2
(2,438)	1:8:A:TYR:HE2	1:23:A:PRO:HG3	3	0.2
(2,402)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	5	0.2
(2,402)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	5	0.2
(2,399)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	6	0.2
(2,362)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,335)	1:22:A:PRO:HA	1:23:A:PRO:HD2	4	0.2
(2,334)	1:22:A:PRO:HA	1:23:A:PRO:HD3	3	0.2
(2,334)	1:22:A:PRO:HA	1:23:A:PRO:HD3	5	0.2
(2,290)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	4	0.2
(2,290)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	7	0.2
(2,290)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	8	0.2
(2,290)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	9	0.2
(2,290)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.2
(2,282)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	1	0.2
(2,282)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	2	0.2
(2,282)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	3	0.2
(2,282)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	5	0.2
(2,282)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	6	0.2
(2,282)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	9	0.2
(2,282)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.2
(2,244)	1:2:A:GLU:HB2	1:5:A:VAL:H	5	0.2
(2,244)	1:2:A:GLU:HB2	1:5:A:VAL:H	8	0.2
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HG	5	0.2
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HG	6	0.2
(2,207)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	1	0.2
(2,207)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	7	0.2
(2,193)	1:11:A:TRP:HE1	1:22:A:PRO:HA	2	0.2
(2,167)	1:19:A:SER:HA	1:19:A:SER:HB2	8	0.2
(2,111)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	5	0.2
(2,102)	1:21:A:ARG:H	1:21:A:ARG:HD2	9	0.2
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG2	9	0.2
(2,101)	1:21:A:ARG:HA	1:21:A:ARG:HG3	9	0.2
(2,94)	1:2:A:GLU:HG2	1:6:A:ARG:H	2	0.2
(2,88)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	3	0.2
(2,65)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	2	0.2
(2,65)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	3	0.2
(2,65)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	4	0.2
(2,65)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	5	0.2
(2,65)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	9	0.2
(2,65)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	10	0.2
(2,64)	1:4:A:CYS:HA	1:4:A:CYS:HB2	1	0.2
(1,728)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	5	0.2
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	1	0.2
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	1	0.2
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	1	0.2
(1,643)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.2
(1,506)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,506)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	2	0.2
(1,506)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	3	0.2
(1,506)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	4	0.2
(1,506)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	5	0.2
(1,506)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	6	0.2
(1,506)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	7	0.2
(1,506)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	9	0.2
(1,357)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	6	0.2
(1,357)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	7	0.2
(1,357)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	8	0.2
(1,357)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.2
(1,318)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	9	0.2
(1,263)	1:19:A:SER:HB2	1:21:A:ARG:H	9	0.2
(1,220)	1:21:A:ARG:HA	1:22:A:PRO:HD2	10	0.2
(1,154)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	1	0.2
(1,154)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	5	0.2
(1,154)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	6	0.2
(1,86)	1:14:A:ASP:H	1:14:A:ASP:HB3	6	0.2
(4,79)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	4	0.19
(4,75)	1:10:A:GLN:HA	1:13:A:LYS:HD2	3	0.19
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	7	0.19
(4,61)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	7	0.19
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	7	0.19
(4,61)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	7	0.19
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	7	0.19
(4,61)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	7	0.19
(4,40)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	1	0.19
(4,40)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	2	0.19
(4,40)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	3	0.19
(4,40)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	4	0.19
(4,40)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	5	0.19
(4,40)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	6	0.19
(4,40)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	7	0.19
(4,40)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	8	0.19
(4,40)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	9	0.19
(4,40)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	10	0.19
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.19
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.19
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.19
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.19
(4,22)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	4	0.19
(4,7)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,7)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	3	0.19
(4,5)	1:14:A:ASP:H	1:14:A:ASP:HB3	3	0.19
(4,5)	1:14:A:ASP:H	1:14:A:ASP:HB3	4	0.19
(4,4)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	1	0.19
(3,647)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	8	0.19
(3,647)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	8	0.19
(3,647)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	8	0.19
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	1	0.19
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	1	0.19
(3,517)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	1	0.19
(3,496)	1:4:A:CYS:HA	1:24:A:PRO:HB2	5	0.19
(3,472)	1:8:A:TYR:HA	1:11:A:TRP:HB2	5	0.19
(3,422)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	4	0.19
(3,422)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	4	0.19
(3,263)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	1	0.19
(3,263)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	3	0.19
(3,263)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	7	0.19
(3,263)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	8	0.19
(3,249)	1:19:A:SER:HB2	1:21:A:ARG:H	8	0.19
(3,210)	1:21:A:ARG:HA	1:22:A:PRO:HD2	1	0.19
(3,210)	1:21:A:ARG:HA	1:22:A:PRO:HD2	2	0.19
(3,93)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.19
(2,745)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	2	0.19
(2,745)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	6	0.19
(2,680)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	4	0.19
(2,680)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	4	0.19
(2,680)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	4	0.19
(2,680)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	9	0.19
(2,680)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	9	0.19
(2,680)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	9	0.19
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	10	0.19
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	10	0.19
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	10	0.19
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	10	0.19
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	10	0.19
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	10	0.19
(2,569)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	3	0.19
(2,569)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	5	0.19
(2,569)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	7	0.19
(2,556)	1:23:A:PRO:HA	1:24:A:PRO:HD3	2	0.19
(2,535)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	10	0.19
(2,522)	1:3:A:GLU:HG2	1:4:A:CYS:HA	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,522)	1:3:A:GLU:HG3	1:4:A:CYS:HA	4	0.19
(2,517)	1:2:A:GLU:HA	1:3:A:GLU:H	6	0.19
(2,515)	1:2:A:GLU:HA	1:2:A:GLU:HB2	8	0.19
(2,494)	1:5:A:VAL:HG21	1:6:A:ARG:HA	2	0.19
(2,494)	1:5:A:VAL:HG22	1:6:A:ARG:HA	2	0.19
(2,494)	1:5:A:VAL:HG23	1:6:A:ARG:HA	2	0.19
(2,466)	1:17:A:PRO:HA	1:18:A:SER:H	10	0.19
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB2	3	0.19
(2,444)	1:10:A:GLN:HE22	1:13:A:LYS:HB3	3	0.19
(2,359)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	7	0.19
(2,334)	1:22:A:PRO:HA	1:23:A:PRO:HD3	4	0.19
(2,334)	1:22:A:PRO:HA	1:23:A:PRO:HD3	8	0.19
(2,307)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	8	0.19
(2,268)	1:11:A:TRP:H	1:12:A:LEU:HA	10	0.19
(2,233)	1:9:A:ILE:H	1:9:A:ILE:HG13	8	0.19
(2,231)	1:7:A:LEU:H	1:7:A:LEU:HG	1	0.19
(2,207)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	4	0.19
(2,207)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	8	0.19
(2,207)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.19
(2,185)	1:20:A:GLY:HA3	1:21:A:ARG:H	1	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG21	4	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG22	4	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG23	4	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG21	6	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG22	6	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG23	6	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG21	7	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG22	7	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG23	7	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG21	8	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG22	8	0.19
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG23	8	0.19
(2,65)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	1	0.19
(2,65)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	6	0.19
(2,65)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	7	0.19
(2,65)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	8	0.19
(2,59)	1:2:A:GLU:HB3	1:4:A:CYS:H	6	0.19
(1,749)	1:7:A:LEU:HB2	1:24:A:PRO:HB2	4	0.19
(1,738)	1:10:A:GLN:HA	1:13:A:LYS:HD2	3	0.19
(1,716)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	8	0.19
(1,716)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	8	0.19
(1,716)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	7	0.19
(1,637)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	7	0.19
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	7	0.19
(1,637)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	7	0.19
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	7	0.19
(1,637)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	7	0.19
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG21	1	0.19
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG22	1	0.19
(1,573)	1:4:A:CYS:HB2	1:5:A:VAL:HG23	1	0.19
(1,546)	1:4:A:CYS:HA	1:24:A:PRO:HB2	5	0.19
(1,519)	1:8:A:TYR:HA	1:11:A:TRP:HB2	5	0.19
(1,504)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	1	0.19
(1,504)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	2	0.19
(1,504)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	3	0.19
(1,504)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	4	0.19
(1,504)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	5	0.19
(1,504)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	6	0.19
(1,504)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	7	0.19
(1,504)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	8	0.19
(1,504)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	9	0.19
(1,504)	1:11:A:TRP:HH2	1:11:A:TRP:HZ2	10	0.19
(1,461)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	4	0.19
(1,461)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	4	0.19
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.19
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.19
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.19
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.19
(1,318)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	4	0.19
(1,280)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	1	0.19
(1,280)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	3	0.19
(1,280)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	7	0.19
(1,280)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	8	0.19
(1,263)	1:19:A:SER:HB2	1:21:A:ARG:H	8	0.19
(1,220)	1:21:A:ARG:HA	1:22:A:PRO:HD2	1	0.19
(1,220)	1:21:A:ARG:HA	1:22:A:PRO:HD2	2	0.19
(1,154)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	2	0.19
(1,154)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	3	0.19
(1,98)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.19
(1,86)	1:14:A:ASP:H	1:14:A:ASP:HB3	3	0.19
(1,86)	1:14:A:ASP:H	1:14:A:ASP:HB3	4	0.19
(1,81)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	1	0.19
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	5	0.18
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	5	0.18
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	4	0.18
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	4	0.18
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	4	0.18
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	6	0.18
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	6	0.18
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	6	0.18
(4,63)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	1	0.18
(4,62)	1:6:A:ARG:HB2	1:7:A:LEU:H	6	0.18
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.18
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.18
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.18
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.18
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.18
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.18
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.18
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.18
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.18
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.18
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.18
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.18
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.18
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.18
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.18
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.18
(4,14)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.18
(4,5)	1:14:A:ASP:H	1:14:A:ASP:HB3	7	0.18
(4,4)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	2	0.18
(4,4)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	5	0.18
(4,4)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	6	0.18
(4,4)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	7	0.18
(4,4)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	8	0.18
(3,655)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	2	0.18
(3,655)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	7	0.18
(3,607)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	4	0.18
(3,607)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	4	0.18
(3,513)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	1	0.18
(3,513)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	5	0.18
(3,513)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	7	0.18
(3,496)	1:4:A:CYS:HA	1:24:A:PRO:HB2	2	0.18
(3,496)	1:4:A:CYS:HA	1:24:A:PRO:HB2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,336)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	4	0.18
(3,336)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	6	0.18
(3,263)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	2	0.18
(3,263)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	4	0.18
(3,263)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	5	0.18
(3,263)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	6	0.18
(3,263)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	9	0.18
(3,256)	1:16:A:GLY:H	1:17:A:PRO:HD2	5	0.18
(3,256)	1:16:A:GLY:H	1:17:A:PRO:HD2	7	0.18
(3,232)	1:7:A:LEU:H	1:10:A:GLN:HB2	1	0.18
(3,222)	1:11:A:TRP:H	1:24:A:PRO:HG2	9	0.18
(3,210)	1:21:A:ARG:HA	1:22:A:PRO:HD2	6	0.18
(3,210)	1:21:A:ARG:HA	1:22:A:PRO:HD2	7	0.18
(3,210)	1:21:A:ARG:HA	1:22:A:PRO:HD2	8	0.18
(3,184)	1:18:A:SER:H	1:19:A:SER:HB2	10	0.18
(3,68)	1:10:A:GLN:H	1:10:A:GLN:HB3	9	0.18
(2,671)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	1	0.18
(2,671)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	1	0.18
(2,671)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	1	0.18
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	2	0.18
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	2	0.18
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	2	0.18
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	2	0.18
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	2	0.18
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	2	0.18
(2,608)	1:6:A:ARG:HA	1:9:A:ILE:HB	7	0.18
(2,556)	1:23:A:PRO:HA	1:24:A:PRO:HD3	3	0.18
(2,556)	1:23:A:PRO:HA	1:24:A:PRO:HD3	5	0.18
(2,556)	1:23:A:PRO:HA	1:24:A:PRO:HD3	6	0.18
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	10	0.18
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	10	0.18
(2,524)	1:4:A:CYS:HA	1:7:A:LEU:HB3	4	0.18
(2,522)	1:3:A:GLU:HG2	1:4:A:CYS:HA	3	0.18
(2,522)	1:3:A:GLU:HG3	1:4:A:CYS:HA	3	0.18
(2,517)	1:2:A:GLU:HA	1:3:A:GLU:H	1	0.18
(2,517)	1:2:A:GLU:HA	1:3:A:GLU:H	4	0.18
(2,517)	1:2:A:GLU:HA	1:3:A:GLU:H	9	0.18
(2,507)	1:11:A:TRP:HA	1:14:A:ASP:HB2	3	0.18
(2,425)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	2	0.18
(2,425)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	2	0.18
(2,359)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	8	0.18
(2,354)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,334)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.18
(2,244)	1:2:A:GLU:HB2	1:5:A:VAL:H	7	0.18
(2,233)	1:9:A:ILE:H	1:9:A:ILE:HG13	4	0.18
(2,233)	1:9:A:ILE:H	1:9:A:ILE:HG13	7	0.18
(2,201)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	1	0.18
(2,201)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	2	0.18
(2,201)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	3	0.18
(2,201)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	5	0.18
(2,201)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	6	0.18
(2,201)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	7	0.18
(2,201)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	8	0.18
(2,201)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	10	0.18
(2,184)	1:19:A:SER:HG	1:21:A:ARG:H	5	0.18
(2,182)	1:18:A:SER:HA	1:19:A:SER:H	1	0.18
(2,182)	1:18:A:SER:HA	1:19:A:SER:H	2	0.18
(2,167)	1:19:A:SER:HA	1:19:A:SER:HB2	4	0.18
(1,728)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	2	0.18
(1,728)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	7	0.18
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD11	5	0.18
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD12	5	0.18
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD13	5	0.18
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	4	0.18
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	4	0.18
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	4	0.18
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	6	0.18
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	6	0.18
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	6	0.18
(1,670)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	4	0.18
(1,670)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	4	0.18
(1,663)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	1	0.18
(1,643)	1:6:A:ARG:HB2	1:7:A:LEU:H	6	0.18
(1,566)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	1	0.18
(1,566)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	5	0.18
(1,566)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	7	0.18
(1,546)	1:4:A:CYS:HA	1:24:A:PRO:HB2	2	0.18
(1,546)	1:4:A:CYS:HA	1:24:A:PRO:HB2	6	0.18
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.18
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.18
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.18
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.18
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.18
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.18
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.18
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.18
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.18
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.18
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.18
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.18
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.18
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.18
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.18
(1,359)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	4	0.18
(1,359)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	6	0.18
(1,280)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	2	0.18
(1,280)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	4	0.18
(1,280)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	5	0.18
(1,280)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	6	0.18
(1,280)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	9	0.18
(1,270)	1:16:A:GLY:H	1:17:A:PRO:HD2	5	0.18
(1,270)	1:16:A:GLY:H	1:17:A:PRO:HD2	7	0.18
(1,262)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.18
(1,244)	1:7:A:LEU:H	1:10:A:GLN:HB2	1	0.18
(1,232)	1:11:A:TRP:H	1:24:A:PRO:HG2	9	0.18
(1,220)	1:21:A:ARG:HA	1:22:A:PRO:HD2	6	0.18
(1,220)	1:21:A:ARG:HA	1:22:A:PRO:HD2	7	0.18
(1,220)	1:21:A:ARG:HA	1:22:A:PRO:HD2	8	0.18
(1,193)	1:18:A:SER:H	1:19:A:SER:HB2	10	0.18
(1,86)	1:14:A:ASP:H	1:14:A:ASP:HB3	7	0.18
(1,81)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	2	0.18
(1,81)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	5	0.18
(1,81)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	6	0.18
(1,81)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	7	0.18
(1,81)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	8	0.18
(1,70)	1:10:A:GLN:H	1:10:A:GLN:HB3	9	0.18
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	2	0.17
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	2	0.17
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	2	0.17
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	4	0.17
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	4	0.17
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	4	0.17
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	6	0.17
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	6	0.17
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	9	0.17
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	9	0.17
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	9	0.17
(4,37)	1:23:A:PRO:HB2	1:25:A:CYS:H	1	0.17
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.17
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.17
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.17
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.17
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.17
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.17
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.17
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.17
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.17
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.17
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.17
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.17
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.17
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.17
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.17
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.17
(4,22)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	10	0.17
(4,5)	1:14:A:ASP:H	1:14:A:ASP:HB3	2	0.17
(4,4)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	3	0.17
(4,4)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	4	0.17
(4,4)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	9	0.17
(4,4)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	10	0.17
(3,513)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	3	0.17
(3,496)	1:4:A:CYS:HA	1:24:A:PRO:HB2	3	0.17
(3,472)	1:8:A:TYR:HA	1:11:A:TRP:HB2	9	0.17
(3,336)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	2	0.17
(3,336)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	3	0.17
(3,336)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	5	0.17
(3,336)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	9	0.17
(3,336)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	0.17
(3,263)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	10	0.17
(3,256)	1:16:A:GLY:H	1:17:A:PRO:HD2	6	0.17
(3,210)	1:21:A:ARG:HA	1:22:A:PRO:HD2	3	0.17
(2,745)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	7	0.17
(2,745)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	9	0.17
(2,741)	1:2:A:GLU:HA	1:5:A:VAL:H	7	0.17
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH21	1	0.17
(2,732)	1:14:A:ASP:HB3	1:21:A:ARG:HH22	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,713)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	4	0.17
(2,713)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	4	0.17
(2,683)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	2	0.17
(2,683)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	2	0.17
(2,683)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	2	0.17
(2,625)	1:19:A:SER:HG	1:20:A:GLY:H	3	0.17
(2,598)	1:21:A:ARG:HB2	1:21:A:ARG:HE	9	0.17
(2,569)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	2	0.17
(2,569)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	6	0.17
(2,556)	1:23:A:PRO:HA	1:24:A:PRO:HD3	4	0.17
(2,518)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	4	0.17
(2,494)	1:5:A:VAL:HG21	1:6:A:ARG:HA	3	0.17
(2,494)	1:5:A:VAL:HG22	1:6:A:ARG:HA	3	0.17
(2,494)	1:5:A:VAL:HG23	1:6:A:ARG:HA	3	0.17
(2,494)	1:5:A:VAL:HG21	1:6:A:ARG:HA	9	0.17
(2,494)	1:5:A:VAL:HG22	1:6:A:ARG:HA	9	0.17
(2,494)	1:5:A:VAL:HG23	1:6:A:ARG:HA	9	0.17
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	8	0.17
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	8	0.17
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	8	0.17
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	8	0.17
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	8	0.17
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	8	0.17
(2,359)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	1	0.17
(2,359)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	2	0.17
(2,359)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	3	0.17
(2,359)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	6	0.17
(2,359)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	9	0.17
(2,354)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	7	0.17
(2,354)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	8	0.17
(2,201)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	4	0.17
(2,201)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	9	0.17
(2,152)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	3	0.17
(2,135)	1:18:A:SER:H	1:18:A:SER:HB3	2	0.17
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD11	2	0.17
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD12	2	0.17
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD13	2	0.17
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD11	4	0.17
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD12	4	0.17
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD13	4	0.17
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD11	6	0.17
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD12	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD13	6	0.17
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD11	9	0.17
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD12	9	0.17
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD13	9	0.17
(1,566)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	3	0.17
(1,546)	1:4:A:CYS:HA	1:24:A:PRO:HB2	3	0.17
(1,519)	1:8:A:TYR:HA	1:11:A:TRP:HB2	9	0.17
(1,443)	1:23:A:PRO:HB2	1:25:A:CYS:H	1	0.17
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.17
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.17
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.17
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.17
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.17
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.17
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.17
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.17
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.17
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.17
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.17
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.17
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.17
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.17
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.17
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.17
(1,359)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	2	0.17
(1,359)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	3	0.17
(1,359)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	5	0.17
(1,359)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	9	0.17
(1,359)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	0.17
(1,318)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	10	0.17
(1,280)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	10	0.17
(1,270)	1:16:A:GLY:H	1:17:A:PRO:HD2	6	0.17
(1,220)	1:21:A:ARG:HA	1:22:A:PRO:HD2	3	0.17
(1,86)	1:14:A:ASP:H	1:14:A:ASP:HB3	2	0.17
(1,81)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	3	0.17
(1,81)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	4	0.17
(1,81)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	9	0.17
(1,81)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	10	0.17
(4,75)	1:10:A:GLN:HA	1:13:A:LYS:HD2	5	0.16
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	3	0.16
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	3	0.16
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	10	0.16
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	10	0.16
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	10	0.16
(4,62)	1:6:A:ARG:HB2	1:7:A:LEU:H	5	0.16
(4,62)	1:6:A:ARG:HB2	1:7:A:LEU:H	8	0.16
(4,37)	1:23:A:PRO:HB2	1:25:A:CYS:H	4	0.16
(4,22)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	2	0.16
(4,22)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	6	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG2	1	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG3	1	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG2	2	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG3	2	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG2	3	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG3	3	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG2	4	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG3	4	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG2	5	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG3	5	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG2	9	0.16
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG3	9	0.16
(4,5)	1:14:A:ASP:H	1:14:A:ASP:HB3	1	0.16
(4,5)	1:14:A:ASP:H	1:14:A:ASP:HB3	9	0.16
(3,607)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	8	0.16
(3,607)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	8	0.16
(3,597)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	1	0.16
(3,597)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	1	0.16
(3,584)	1:10:A:GLN:HA	1:13:A:LYS:H	1	0.16
(3,545)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	9	0.16
(3,513)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	6	0.16
(3,513)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	10	0.16
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB2	3	0.16
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB3	3	0.16
(3,472)	1:8:A:TYR:HA	1:11:A:TRP:HB2	3	0.16
(3,336)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	7	0.16
(3,256)	1:16:A:GLY:H	1:17:A:PRO:HD2	2	0.16
(3,222)	1:11:A:TRP:H	1:24:A:PRO:HG2	4	0.16
(3,86)	1:4:A:CYS:HB2	1:5:A:VAL:H	8	0.16
(2,745)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	8	0.16
(2,745)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	10	0.16
(2,737)	1:12:A:LEU:HB3	1:14:A:ASP:H	1	0.16
(2,737)	1:12:A:LEU:HB3	1:14:A:ASP:H	6	0.16
(2,644)	1:8:A:TYR:HE1	1:11:A:TRP:HZ3	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,644)	1:8:A:TYR:HE2	1:11:A:TRP:HZ3	3	0.16
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	5	0.16
(2,631)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	5	0.16
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	5	0.16
(2,631)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	5	0.16
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	5	0.16
(2,631)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	5	0.16
(2,582)	1:7:A:LEU:HG	1:8:A:TYR:H	1	0.16
(2,569)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	10	0.16
(2,522)	1:3:A:GLU:HG2	1:4:A:CYS:HA	10	0.16
(2,522)	1:3:A:GLU:HG3	1:4:A:CYS:HA	10	0.16
(2,518)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	6	0.16
(2,517)	1:2:A:GLU:HA	1:3:A:GLU:H	5	0.16
(2,494)	1:5:A:VAL:HG21	1:6:A:ARG:HA	10	0.16
(2,494)	1:5:A:VAL:HG22	1:6:A:ARG:HA	10	0.16
(2,494)	1:5:A:VAL:HG23	1:6:A:ARG:HA	10	0.16
(2,459)	1:14:A:ASP:HB2	1:15:A:GLY:H	10	0.16
(2,426)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	9	0.16
(2,426)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	9	0.16
(2,426)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	10	0.16
(2,426)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	10	0.16
(2,425)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	3	0.16
(2,425)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	3	0.16
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	7	0.16
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	7	0.16
(2,415)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	7	0.16
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	7	0.16
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	7	0.16
(2,415)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	7	0.16
(2,394)	1:8:A:TYR:HE1	1:24:A:PRO:HD2	4	0.16
(2,394)	1:8:A:TYR:HE2	1:24:A:PRO:HD2	4	0.16
(2,359)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	4	0.16
(2,359)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	5	0.16
(2,359)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	10	0.16
(2,354)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	2	0.16
(2,354)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	4	0.16
(2,354)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	5	0.16
(2,354)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	6	0.16
(2,354)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	9	0.16
(2,345)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	3	0.16
(2,345)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	6	0.16
(2,345)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,334)	1:22:A:PRO:HA	1:23:A:PRO:HD3	1	0.16
(2,329)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	8	0.16
(2,307)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	10	0.16
(2,273)	1:11:A:TRP:HE1	1:19:A:SER:HB3	10	0.16
(2,233)	1:9:A:ILE:H	1:9:A:ILE:HG13	3	0.16
(2,231)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.16
(2,218)	1:13:A:LYS:H	1:13:A:LYS:HB2	10	0.16
(2,218)	1:13:A:LYS:H	1:13:A:LYS:HB3	10	0.16
(2,183)	1:19:A:SER:H	1:19:A:SER:HG	6	0.16
(2,138)	1:18:A:SER:HA	1:18:A:SER:HB2	8	0.16
(2,135)	1:18:A:SER:H	1:18:A:SER:HB3	1	0.16
(2,131)	1:20:A:GLY:H	1:20:A:GLY:HA2	10	0.16
(2,71)	1:5:A:VAL:H	1:5:A:VAL:HB	7	0.16
(1,738)	1:10:A:GLN:HA	1:13:A:LYS:HD2	5	0.16
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD11	3	0.16
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD12	3	0.16
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD13	3	0.16
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD11	10	0.16
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD12	10	0.16
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD13	10	0.16
(1,670)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	8	0.16
(1,670)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	8	0.16
(1,659)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	1	0.16
(1,659)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	1	0.16
(1,646)	1:10:A:GLN:HA	1:13:A:LYS:H	1	0.16
(1,643)	1:6:A:ARG:HB2	1:7:A:LEU:H	5	0.16
(1,643)	1:6:A:ARG:HB2	1:7:A:LEU:H	8	0.16
(1,601)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	9	0.16
(1,566)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	6	0.16
(1,566)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	10	0.16
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB2	3	0.16
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB3	3	0.16
(1,519)	1:8:A:TYR:HA	1:11:A:TRP:HB2	3	0.16
(1,443)	1:23:A:PRO:HB2	1:25:A:CYS:H	4	0.16
(1,359)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	7	0.16
(1,318)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	2	0.16
(1,318)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	6	0.16
(1,270)	1:16:A:GLY:H	1:17:A:PRO:HD2	2	0.16
(1,232)	1:11:A:TRP:H	1:24:A:PRO:HG2	4	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG2	1	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG3	1	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG2	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG3	2	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG2	3	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG3	3	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG2	4	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG3	4	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG2	5	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG3	5	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG2	9	0.16
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG3	9	0.16
(1,91)	1:4:A:CYS:HB2	1:5:A:VAL:H	8	0.16
(1,86)	1:14:A:ASP:H	1:14:A:ASP:HB3	1	0.16
(1,86)	1:14:A:ASP:H	1:14:A:ASP:HB3	9	0.16
(4,75)	1:10:A:GLN:HA	1:13:A:LYS:HD2	8	0.15
(4,75)	1:10:A:GLN:HA	1:13:A:LYS:HD2	9	0.15
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	7	0.15
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	7	0.15
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	7	0.15
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	8	0.15
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	8	0.15
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	8	0.15
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	1	0.15
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	1	0.15
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	1	0.15
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.15
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.15
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.15
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	3	0.15
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	3	0.15
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	3	0.15
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.15
(4,26)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.15
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.15
(4,26)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.15
(4,22)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	1	0.15
(4,22)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	5	0.15
(4,22)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	8	0.15
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG2	6	0.15
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG3	6	0.15
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG2	7	0.15
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG3	7	0.15
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG2	8	0.15
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG3	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG2	10	0.15
(4,8)	1:3:A:GLU:HA	1:3:A:GLU:HG3	10	0.15
(3,655)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	3	0.15
(3,648)	1:2:A:GLU:HB2	1:5:A:VAL:HG21	2	0.15
(3,648)	1:2:A:GLU:HB2	1:5:A:VAL:HG22	2	0.15
(3,648)	1:2:A:GLU:HB2	1:5:A:VAL:HG23	2	0.15
(3,513)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	4	0.15
(3,513)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	9	0.15
(3,496)	1:4:A:CYS:HA	1:24:A:PRO:HB2	9	0.15
(3,496)	1:4:A:CYS:HA	1:24:A:PRO:HB2	10	0.15
(3,472)	1:8:A:TYR:HA	1:11:A:TRP:HB2	10	0.15
(3,440)	1:15:A:GLY:HA3	1:16:A:GLY:H	5	0.15
(3,419)	1:8:A:TYR:HE1	1:12:A:LEU:HG	4	0.15
(3,419)	1:8:A:TYR:HE2	1:12:A:LEU:HG	4	0.15
(3,416)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	1	0.15
(3,416)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	3	0.15
(3,416)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	4	0.15
(3,416)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	6	0.15
(3,416)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	7	0.15
(3,256)	1:16:A:GLY:H	1:17:A:PRO:HD2	3	0.15
(3,256)	1:16:A:GLY:H	1:17:A:PRO:HD2	4	0.15
(3,256)	1:16:A:GLY:H	1:17:A:PRO:HD2	9	0.15
(3,203)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	1	0.15
(3,203)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	7	0.15
(3,184)	1:18:A:SER:H	1:19:A:SER:HB2	3	0.15
(3,58)	1:2:A:GLU:HB3	1:4:A:CYS:H	2	0.15
(2,745)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	1	0.15
(2,745)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	3	0.15
(2,745)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	4	0.15
(2,744)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	4	0.15
(2,744)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	5	0.15
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD11	4	0.15
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD12	4	0.15
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD13	4	0.15
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD21	4	0.15
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD22	4	0.15
(2,672)	1:4:A:CYS:HB2	1:7:A:LEU:HD23	4	0.15
(2,644)	1:8:A:TYR:HE1	1:11:A:TRP:HZ3	10	0.15
(2,644)	1:8:A:TYR:HE2	1:11:A:TRP:HZ3	10	0.15
(2,576)	1:6:A:ARG:H	1:8:A:TYR:H	9	0.15
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	2	0.15
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	2	0.15
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	2	0.15
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	2	0.15
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	2	0.15
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	5	0.15
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	5	0.15
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	5	0.15
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	5	0.15
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	5	0.15
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	5	0.15
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	7	0.15
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	7	0.15
(2,522)	1:3:A:GLU:HG2	1:4:A:CYS:HA	9	0.15
(2,522)	1:3:A:GLU:HG3	1:4:A:CYS:HA	9	0.15
(2,518)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	1	0.15
(2,518)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	3	0.15
(2,518)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	5	0.15
(2,518)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	7	0.15
(2,518)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	8	0.15
(2,518)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	9	0.15
(2,518)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	10	0.15
(2,511)	1:14:A:ASP:HB2	1:19:A:SER:HB2	5	0.15
(2,494)	1:5:A:VAL:HG21	1:6:A:ARG:HA	5	0.15
(2,494)	1:5:A:VAL:HG22	1:6:A:ARG:HA	5	0.15
(2,494)	1:5:A:VAL:HG23	1:6:A:ARG:HA	5	0.15
(2,452)	1:11:A:TRP:HE3	1:23:A:PRO:HA	3	0.15
(2,452)	1:11:A:TRP:HE3	1:23:A:PRO:HA	8	0.15
(2,432)	1:11:A:TRP:HD1	1:21:A:ARG:HG2	9	0.15
(2,432)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	9	0.15
(2,425)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	7	0.15
(2,425)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	7	0.15
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	1	0.15
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	1	0.15
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	1	0.15
(2,399)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	3	0.15
(2,376)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	6	0.15
(2,354)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	3	0.15
(2,354)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	10	0.15
(2,345)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	1	0.15
(2,345)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	2	0.15
(2,345)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	4	0.15
(2,345)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,345)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	7	0.15
(2,345)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	8	0.15
(2,345)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	9	0.15
(2,334)	1:22:A:PRO:HA	1:23:A:PRO:HD3	7	0.15
(2,334)	1:22:A:PRO:HA	1:23:A:PRO:HD3	9	0.15
(2,329)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	1	0.15
(2,329)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	2	0.15
(2,329)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	3	0.15
(2,329)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	5	0.15
(2,329)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	6	0.15
(2,329)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	7	0.15
(2,329)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.15
(2,307)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	6	0.15
(2,304)	1:17:A:PRO:HA	1:17:A:PRO:HB3	4	0.15
(2,304)	1:17:A:PRO:HA	1:17:A:PRO:HB3	6	0.15
(2,304)	1:17:A:PRO:HA	1:17:A:PRO:HB3	8	0.15
(2,304)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.15
(2,300)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	2	0.15
(2,300)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	4	0.15
(2,300)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	9	0.15
(2,295)	1:12:A:LEU:HD11	1:12:A:LEU:HG	1	0.15
(2,295)	1:12:A:LEU:HD12	1:12:A:LEU:HG	1	0.15
(2,295)	1:12:A:LEU:HD13	1:12:A:LEU:HG	1	0.15
(2,295)	1:12:A:LEU:HD11	1:12:A:LEU:HG	2	0.15
(2,295)	1:12:A:LEU:HD12	1:12:A:LEU:HG	2	0.15
(2,295)	1:12:A:LEU:HD13	1:12:A:LEU:HG	2	0.15
(2,295)	1:12:A:LEU:HD11	1:12:A:LEU:HG	3	0.15
(2,295)	1:12:A:LEU:HD12	1:12:A:LEU:HG	3	0.15
(2,295)	1:12:A:LEU:HD13	1:12:A:LEU:HG	3	0.15
(2,295)	1:12:A:LEU:HD11	1:12:A:LEU:HG	4	0.15
(2,295)	1:12:A:LEU:HD12	1:12:A:LEU:HG	4	0.15
(2,295)	1:12:A:LEU:HD13	1:12:A:LEU:HG	4	0.15
(2,295)	1:12:A:LEU:HD11	1:12:A:LEU:HG	5	0.15
(2,295)	1:12:A:LEU:HD12	1:12:A:LEU:HG	5	0.15
(2,295)	1:12:A:LEU:HD13	1:12:A:LEU:HG	5	0.15
(2,295)	1:12:A:LEU:HD11	1:12:A:LEU:HG	6	0.15
(2,295)	1:12:A:LEU:HD12	1:12:A:LEU:HG	6	0.15
(2,295)	1:12:A:LEU:HD13	1:12:A:LEU:HG	6	0.15
(2,295)	1:12:A:LEU:HD11	1:12:A:LEU:HG	7	0.15
(2,295)	1:12:A:LEU:HD12	1:12:A:LEU:HG	7	0.15
(2,295)	1:12:A:LEU:HD13	1:12:A:LEU:HG	7	0.15
(2,295)	1:12:A:LEU:HD11	1:12:A:LEU:HG	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,295)	1:12:A:LEU:HD12	1:12:A:LEU:HG	8	0.15
(2,295)	1:12:A:LEU:HD13	1:12:A:LEU:HG	8	0.15
(2,295)	1:12:A:LEU:HD11	1:12:A:LEU:HG	9	0.15
(2,295)	1:12:A:LEU:HD12	1:12:A:LEU:HG	9	0.15
(2,295)	1:12:A:LEU:HD13	1:12:A:LEU:HG	9	0.15
(2,295)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.15
(2,295)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.15
(2,295)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.15
(2,263)	1:9:A:ILE:HA	1:12:A:LEU:H	10	0.15
(2,233)	1:9:A:ILE:H	1:9:A:ILE:HG13	6	0.15
(2,231)	1:7:A:LEU:H	1:7:A:LEU:HG	9	0.15
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG21	3	0.15
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG22	3	0.15
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG23	3	0.15
(2,152)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	2	0.15
(2,138)	1:18:A:SER:HA	1:18:A:SER:HB2	2	0.15
(2,138)	1:18:A:SER:HA	1:18:A:SER:HB2	10	0.15
(2,110)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	8	0.15
(2,87)	1:14:A:ASP:HA	1:14:A:ASP:HB2	10	0.15
(2,71)	1:5:A:VAL:H	1:5:A:VAL:HB	8	0.15
(2,61)	1:4:A:CYS:H	1:4:A:CYS:HB3	1	0.15
(2,61)	1:4:A:CYS:H	1:4:A:CYS:HB3	3	0.15
(2,61)	1:4:A:CYS:H	1:4:A:CYS:HB3	5	0.15
(1,738)	1:10:A:GLN:HA	1:13:A:LYS:HD2	8	0.15
(1,738)	1:10:A:GLN:HA	1:13:A:LYS:HD2	9	0.15
(1,728)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	3	0.15
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD11	7	0.15
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD12	7	0.15
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD13	7	0.15
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD11	8	0.15
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD12	8	0.15
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD13	8	0.15
(1,718)	1:2:A:GLU:HB2	1:5:A:VAL:HG21	2	0.15
(1,718)	1:2:A:GLU:HB2	1:5:A:VAL:HG22	2	0.15
(1,718)	1:2:A:GLU:HB2	1:5:A:VAL:HG23	2	0.15
(1,566)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	4	0.15
(1,566)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	9	0.15
(1,546)	1:4:A:CYS:HA	1:24:A:PRO:HB2	9	0.15
(1,546)	1:4:A:CYS:HA	1:24:A:PRO:HB2	10	0.15
(1,519)	1:8:A:TYR:HA	1:11:A:TRP:HB2	10	0.15
(1,479)	1:15:A:GLY:HA3	1:16:A:GLY:H	5	0.15
(1,458)	1:8:A:TYR:HE1	1:12:A:LEU:HG	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:8:A:TYR:HE2	1:12:A:LEU:HG	4	0.15
(1,455)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	1	0.15
(1,455)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	3	0.15
(1,455)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	4	0.15
(1,455)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	6	0.15
(1,455)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	7	0.15
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	1	0.15
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	1	0.15
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	1	0.15
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.15
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.15
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.15
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	3	0.15
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	3	0.15
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	3	0.15
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.15
(1,398)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.15
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.15
(1,398)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.15
(1,318)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	1	0.15
(1,318)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	5	0.15
(1,318)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	8	0.15
(1,270)	1:16:A:GLY:H	1:17:A:PRO:HD2	3	0.15
(1,270)	1:16:A:GLY:H	1:17:A:PRO:HD2	4	0.15
(1,270)	1:16:A:GLY:H	1:17:A:PRO:HD2	9	0.15
(1,213)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	1	0.15
(1,213)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	7	0.15
(1,193)	1:18:A:SER:H	1:19:A:SER:HB2	3	0.15
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG2	6	0.15
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG3	6	0.15
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG2	7	0.15
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG3	7	0.15
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG2	8	0.15
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG3	8	0.15
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG2	10	0.15
(1,176)	1:3:A:GLU:HA	1:3:A:GLU:HG3	10	0.15
(1,60)	1:2:A:GLU:HB3	1:4:A:CYS:H	2	0.15
(4,75)	1:10:A:GLN:HA	1:13:A:LYS:HD2	4	0.14
(4,75)	1:10:A:GLN:HA	1:13:A:LYS:HD2	7	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	4	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	4	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	5	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	5	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	5	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	6	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	6	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	6	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	7	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	7	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	7	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	8	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	8	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	8	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	9	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	9	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	9	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.14
(4,32)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.14
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	5	0.14
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	5	0.14
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	5	0.14
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	9	0.14
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	9	0.14
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	9	0.14
(4,22)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	3	0.14
(3,655)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	6	0.14
(3,655)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	9	0.14
(3,647)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	2	0.14
(3,647)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	2	0.14
(3,647)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	2	0.14
(3,647)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	5	0.14
(3,647)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	5	0.14
(3,647)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	5	0.14
(3,647)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	9	0.14
(3,647)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	9	0.14
(3,647)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	9	0.14
(3,620)	1:7:A:LEU:HD11	1:25:A:CYS:HA	10	0.14
(3,620)	1:7:A:LEU:HD12	1:25:A:CYS:HA	10	0.14
(3,620)	1:7:A:LEU:HD13	1:25:A:CYS:HA	10	0.14
(3,620)	1:7:A:LEU:HD21	1:25:A:CYS:HA	10	0.14
(3,620)	1:7:A:LEU:HD22	1:25:A:CYS:HA	10	0.14
(3,620)	1:7:A:LEU:HD23	1:25:A:CYS:HA	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,607)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	2	0.14
(3,607)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	2	0.14
(3,573)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	3	0.14
(3,513)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	8	0.14
(3,509)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	9	0.14
(3,509)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	9	0.14
(3,496)	1:4:A:CYS:HA	1:24:A:PRO:HB2	4	0.14
(3,478)	1:14:A:ASP:HB3	1:19:A:SER:HB2	10	0.14
(3,440)	1:15:A:GLY:HA3	1:16:A:GLY:H	3	0.14
(3,416)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	5	0.14
(3,416)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	8	0.14
(3,336)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	8	0.14
(3,256)	1:16:A:GLY:H	1:17:A:PRO:HD2	1	0.14
(3,256)	1:16:A:GLY:H	1:17:A:PRO:HD2	8	0.14
(3,249)	1:19:A:SER:HB2	1:21:A:ARG:H	10	0.14
(3,222)	1:11:A:TRP:H	1:24:A:PRO:HG2	2	0.14
(3,222)	1:11:A:TRP:H	1:24:A:PRO:HG2	5	0.14
(3,203)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	10	0.14
(3,93)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.14
(3,86)	1:4:A:CYS:HB2	1:5:A:VAL:H	7	0.14
(3,68)	1:10:A:GLN:H	1:10:A:GLN:HB3	7	0.14
(3,66)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.14
(3,29)	1:5:A:VAL:H	1:5:A:VAL:HG21	4	0.14
(3,29)	1:5:A:VAL:H	1:5:A:VAL:HG22	4	0.14
(3,29)	1:5:A:VAL:H	1:5:A:VAL:HG23	4	0.14
(3,14)	1:5:A:VAL:H	1:5:A:VAL:HG21	4	0.14
(3,14)	1:5:A:VAL:H	1:5:A:VAL:HG22	4	0.14
(3,14)	1:5:A:VAL:H	1:5:A:VAL:HG23	4	0.14
(2,745)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	5	0.14
(2,744)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	1	0.14
(2,744)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	3	0.14
(2,744)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	8	0.14
(2,744)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	10	0.14
(2,675)	1:12:A:LEU:HB3	1:13:A:LYS:HD2	8	0.14
(2,576)	1:6:A:ARG:H	1:8:A:TYR:H	1	0.14
(2,576)	1:6:A:ARG:H	1:8:A:TYR:H	5	0.14
(2,576)	1:6:A:ARG:H	1:8:A:TYR:H	10	0.14
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	6	0.14
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	6	0.14
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	6	0.14
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	6	0.14
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	6	0.14
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	10	0.14
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	10	0.14
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	10	0.14
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	10	0.14
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	10	0.14
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	10	0.14
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	3	0.14
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	3	0.14
(2,518)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	2	0.14
(2,511)	1:14:A:ASP:HB2	1:19:A:SER:HB2	1	0.14
(2,507)	1:11:A:TRP:HA	1:14:A:ASP:HB2	6	0.14
(2,466)	1:17:A:PRO:HA	1:18:A:SER:H	8	0.14
(2,452)	1:11:A:TRP:HE3	1:23:A:PRO:HA	9	0.14
(2,402)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	9	0.14
(2,402)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	9	0.14
(2,329)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	9	0.14
(2,304)	1:17:A:PRO:HA	1:17:A:PRO:HB3	2	0.14
(2,304)	1:17:A:PRO:HA	1:17:A:PRO:HB3	3	0.14
(2,304)	1:17:A:PRO:HA	1:17:A:PRO:HB3	9	0.14
(2,300)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	1	0.14
(2,300)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	3	0.14
(2,300)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	5	0.14
(2,300)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	6	0.14
(2,300)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	8	0.14
(2,300)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.14
(2,246)	1:7:A:LEU:HG	1:25:A:CYS:H	2	0.14
(2,244)	1:2:A:GLU:HB2	1:5:A:VAL:H	1	0.14
(2,233)	1:9:A:ILE:H	1:9:A:ILE:HG13	5	0.14
(2,218)	1:13:A:LYS:H	1:13:A:LYS:HB2	6	0.14
(2,218)	1:13:A:LYS:H	1:13:A:LYS:HB3	6	0.14
(2,186)	1:19:A:SER:HA	1:19:A:SER:HG	4	0.14
(2,185)	1:20:A:GLY:HA3	1:21:A:ARG:H	7	0.14
(2,167)	1:19:A:SER:HA	1:19:A:SER:HB2	6	0.14
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG21	2	0.14
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG22	2	0.14
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG23	2	0.14
(2,152)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	1	0.14
(2,138)	1:18:A:SER:HA	1:18:A:SER:HB2	1	0.14
(2,131)	1:20:A:GLY:H	1:20:A:GLY:HA2	3	0.14
(2,92)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	3	0.14
(2,92)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,92)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	7	0.14
(2,71)	1:5:A:VAL:H	1:5:A:VAL:HB	5	0.14
(2,61)	1:4:A:CYS:H	1:4:A:CYS:HB3	2	0.14
(2,59)	1:2:A:GLU:HB3	1:4:A:CYS:H	4	0.14
(1,738)	1:10:A:GLN:HA	1:13:A:LYS:HD2	4	0.14
(1,738)	1:10:A:GLN:HA	1:13:A:LYS:HD2	7	0.14
(1,728)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	6	0.14
(1,728)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	9	0.14
(1,716)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	2	0.14
(1,716)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	2	0.14
(1,716)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	2	0.14
(1,716)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	5	0.14
(1,716)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	5	0.14
(1,716)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	5	0.14
(1,716)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	9	0.14
(1,716)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	9	0.14
(1,716)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	9	0.14
(1,686)	1:7:A:LEU:HD11	1:25:A:CYS:HA	10	0.14
(1,686)	1:7:A:LEU:HD12	1:25:A:CYS:HA	10	0.14
(1,686)	1:7:A:LEU:HD13	1:25:A:CYS:HA	10	0.14
(1,686)	1:7:A:LEU:HD21	1:25:A:CYS:HA	10	0.14
(1,686)	1:7:A:LEU:HD22	1:25:A:CYS:HA	10	0.14
(1,686)	1:7:A:LEU:HD23	1:25:A:CYS:HA	10	0.14
(1,670)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	2	0.14
(1,670)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	2	0.14
(1,632)	1:10:A:GLN:HB3	1:11:A:TRP:HB3	3	0.14
(1,566)	1:11:A:TRP:HB3	1:24:A:PRO:HG2	8	0.14
(1,561)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	9	0.14
(1,561)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	9	0.14
(1,546)	1:4:A:CYS:HA	1:24:A:PRO:HB2	4	0.14
(1,525)	1:14:A:ASP:HB3	1:19:A:SER:HB2	10	0.14
(1,479)	1:15:A:GLY:HA3	1:16:A:GLY:H	3	0.14
(1,455)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	5	0.14
(1,455)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	8	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	4	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	4	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	4	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	5	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	5	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	5	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	6	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	6	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	7	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	7	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	7	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	8	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	8	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	8	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	9	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	9	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	9	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.14
(1,428)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.14
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	5	0.14
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	5	0.14
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	5	0.14
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	9	0.14
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	9	0.14
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	9	0.14
(1,359)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	8	0.14
(1,318)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	3	0.14
(1,270)	1:16:A:GLY:H	1:17:A:PRO:HD2	1	0.14
(1,270)	1:16:A:GLY:H	1:17:A:PRO:HD2	8	0.14
(1,263)	1:19:A:SER:HB2	1:21:A:ARG:H	10	0.14
(1,232)	1:11:A:TRP:H	1:24:A:PRO:HG2	2	0.14
(1,232)	1:11:A:TRP:H	1:24:A:PRO:HG2	5	0.14
(1,213)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	10	0.14
(1,98)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.14
(1,91)	1:4:A:CYS:HB2	1:5:A:VAL:H	7	0.14
(1,70)	1:10:A:GLN:H	1:10:A:GLN:HB3	7	0.14
(1,68)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.14
(1,31)	1:5:A:VAL:H	1:5:A:VAL:HG21	4	0.14
(1,31)	1:5:A:VAL:H	1:5:A:VAL:HG22	4	0.14
(1,31)	1:5:A:VAL:H	1:5:A:VAL:HG23	4	0.14
(1,15)	1:5:A:VAL:H	1:5:A:VAL:HG21	4	0.14
(1,15)	1:5:A:VAL:H	1:5:A:VAL:HG22	4	0.14
(1,15)	1:5:A:VAL:H	1:5:A:VAL:HG23	4	0.14
(4,45)	1:4:A:CYS:HA	1:7:A:LEU:HB2	1	0.13
(4,45)	1:4:A:CYS:HA	1:7:A:LEU:HB2	8	0.13
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	3	0.13
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	3	0.13
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	6	0.13
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	6	0.13
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	6	0.13
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	10	0.13
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	10	0.13
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	10	0.13
(4,19)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.13
(3,655)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	1	0.13
(3,647)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	10	0.13
(3,647)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	10	0.13
(3,647)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	10	0.13
(3,607)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	1	0.13
(3,607)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	1	0.13
(3,597)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	7	0.13
(3,597)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	7	0.13
(3,472)	1:8:A:TYR:HA	1:11:A:TRP:HB2	7	0.13
(3,416)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	9	0.13
(3,416)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	0.13
(3,411)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	10	0.13
(3,336)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	1	0.13
(3,256)	1:16:A:GLY:H	1:17:A:PRO:HD2	10	0.13
(3,222)	1:11:A:TRP:H	1:24:A:PRO:HG2	6	0.13
(3,212)	1:21:A:ARG:HA	1:22:A:PRO:HG2	9	0.13
(3,210)	1:21:A:ARG:HA	1:22:A:PRO:HD2	5	0.13
(3,203)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	2	0.13
(3,203)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	8	0.13
(3,179)	1:19:A:SER:H	1:19:A:SER:HG	4	0.13
(3,93)	1:21:A:ARG:H	1:21:A:ARG:HB3	1	0.13
(3,93)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.13
(3,93)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.13
(3,91)	1:2:A:GLU:HG2	1:5:A:VAL:H	4	0.13
(3,71)	1:5:A:VAL:HB	1:6:A:ARG:H	8	0.13
(2,654)	1:3:A:GLU:HA	1:6:A:ARG:HB2	4	0.13
(2,576)	1:6:A:ARG:H	1:8:A:TYR:H	3	0.13
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	3	0.13
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	3	0.13
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	3	0.13
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	3	0.13
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	3	0.13
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	3	0.13
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	8	0.13
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,517)	1:2:A:GLU:HA	1:3:A:GLU:H	10	0.13
(2,507)	1:11:A:TRP:HA	1:14:A:ASP:HB2	9	0.13
(2,494)	1:5:A:VAL:HG21	1:6:A:ARG:HA	1	0.13
(2,494)	1:5:A:VAL:HG22	1:6:A:ARG:HA	1	0.13
(2,494)	1:5:A:VAL:HG23	1:6:A:ARG:HA	1	0.13
(2,467)	1:18:A:SER:HA	1:20:A:GLY:H	3	0.13
(2,394)	1:8:A:TYR:HE1	1:24:A:PRO:HD2	7	0.13
(2,394)	1:8:A:TYR:HE2	1:24:A:PRO:HD2	7	0.13
(2,368)	1:8:A:TYR:HD1	1:9:A:ILE:HA	1	0.13
(2,368)	1:8:A:TYR:HD2	1:9:A:ILE:HA	1	0.13
(2,362)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	8	0.13
(2,360)	1:11:A:TRP:HD1	1:19:A:SER:HG	6	0.13
(2,351)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	2	0.13
(2,351)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	3	0.13
(2,351)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	4	0.13
(2,351)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	5	0.13
(2,351)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	7	0.13
(2,351)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	8	0.13
(2,351)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	9	0.13
(2,351)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	10	0.13
(2,329)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	4	0.13
(2,304)	1:17:A:PRO:HA	1:17:A:PRO:HB3	1	0.13
(2,304)	1:17:A:PRO:HA	1:17:A:PRO:HB3	5	0.13
(2,304)	1:17:A:PRO:HA	1:17:A:PRO:HB3	7	0.13
(2,300)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	7	0.13
(2,250)	1:19:A:SER:HA	1:20:A:GLY:H	3	0.13
(2,250)	1:19:A:SER:HA	1:20:A:GLY:H	10	0.13
(2,242)	1:17:A:PRO:HB2	1:18:A:SER:H	10	0.13
(2,233)	1:9:A:ILE:H	1:9:A:ILE:HG13	9	0.13
(2,231)	1:7:A:LEU:H	1:7:A:LEU:HG	2	0.13
(2,225)	1:14:A:ASP:H	1:15:A:GLY:H	10	0.13
(2,218)	1:13:A:LYS:H	1:13:A:LYS:HB2	2	0.13
(2,218)	1:13:A:LYS:H	1:13:A:LYS:HB3	2	0.13
(2,184)	1:19:A:SER:HG	1:21:A:ARG:H	2	0.13
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG21	5	0.13
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG22	5	0.13
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG23	5	0.13
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG21	9	0.13
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG22	9	0.13
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG23	9	0.13
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG21	10	0.13
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG22	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,160)	1:5:A:VAL:HA	1:5:A:VAL:HG23	10	0.13
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG21	4	0.13
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG22	4	0.13
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG23	4	0.13
(2,92)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	1	0.13
(2,92)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	2	0.13
(2,84)	1:14:A:ASP:H	1:14:A:ASP:HB2	9	0.13
(2,71)	1:5:A:VAL:H	1:5:A:VAL:HB	3	0.13
(2,71)	1:5:A:VAL:H	1:5:A:VAL:HB	10	0.13
(2,61)	1:4:A:CYS:H	1:4:A:CYS:HB3	9	0.13
(1,728)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	1	0.13
(1,716)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	10	0.13
(1,716)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	10	0.13
(1,716)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	10	0.13
(1,670)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	1	0.13
(1,670)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	1	0.13
(1,659)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	7	0.13
(1,659)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	7	0.13
(1,519)	1:8:A:TYR:HA	1:11:A:TRP:HB2	7	0.13
(1,514)	1:4:A:CYS:HA	1:7:A:LEU:HB2	1	0.13
(1,514)	1:4:A:CYS:HA	1:7:A:LEU:HB2	8	0.13
(1,455)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	9	0.13
(1,455)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	0.13
(1,448)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	10	0.13
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	3	0.13
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	3	0.13
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	3	0.13
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	6	0.13
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	6	0.13
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	6	0.13
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	10	0.13
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	10	0.13
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	10	0.13
(1,359)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	1	0.13
(1,291)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.13
(1,270)	1:16:A:GLY:H	1:17:A:PRO:HD2	10	0.13
(1,232)	1:11:A:TRP:H	1:24:A:PRO:HG2	6	0.13
(1,222)	1:21:A:ARG:HA	1:22:A:PRO:HG2	9	0.13
(1,220)	1:21:A:ARG:HA	1:22:A:PRO:HD2	5	0.13
(1,213)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	2	0.13
(1,213)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	8	0.13
(1,187)	1:19:A:SER:H	1:19:A:SER:HG	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:21:A:ARG:H	1:21:A:ARG:HB3	1	0.13
(1,98)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.13
(1,98)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.13
(1,96)	1:2:A:GLU:HG2	1:5:A:VAL:H	4	0.13
(1,73)	1:5:A:VAL:HB	1:6:A:ARG:H	8	0.13
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	1	0.12
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	1	0.12
(4,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	1	0.12
(4,63)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	4	0.12
(4,45)	1:4:A:CYS:HA	1:7:A:LEU:HB2	7	0.12
(4,37)	1:23:A:PRO:HB2	1:25:A:CYS:H	2	0.12
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	2	0.12
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	2	0.12
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	2	0.12
(4,22)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	7	0.12
(3,647)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	3	0.12
(3,647)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	3	0.12
(3,647)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	3	0.12
(3,607)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	5	0.12
(3,607)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	5	0.12
(3,416)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	2	0.12
(3,410)	1:11:A:TRP:HD1	1:21:A:ARG:HG2	8	0.12
(3,410)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	8	0.12
(3,289)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	1	0.12
(3,289)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	3	0.12
(3,289)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	5	0.12
(3,289)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	7	0.12
(3,227)	1:6:A:ARG:HG2	1:7:A:LEU:H	8	0.12
(3,210)	1:21:A:ARG:HA	1:22:A:PRO:HD2	9	0.12
(3,184)	1:18:A:SER:H	1:19:A:SER:HB2	1	0.12
(3,184)	1:18:A:SER:H	1:19:A:SER:HB2	2	0.12
(3,179)	1:19:A:SER:H	1:19:A:SER:HG	10	0.12
(3,105)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	5	0.12
(3,71)	1:5:A:VAL:HB	1:6:A:ARG:H	1	0.12
(3,68)	1:10:A:GLN:H	1:10:A:GLN:HB3	4	0.12
(3,66)	1:10:A:GLN:H	1:10:A:GLN:HG3	1	0.12
(3,66)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.12
(3,33)	1:6:A:ARG:H	1:6:A:ARG:HG3	1	0.12
(3,29)	1:5:A:VAL:H	1:5:A:VAL:HG21	6	0.12
(3,29)	1:5:A:VAL:H	1:5:A:VAL:HG22	6	0.12
(3,29)	1:5:A:VAL:H	1:5:A:VAL:HG23	6	0.12
(3,14)	1:5:A:VAL:H	1:5:A:VAL:HG21	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,14)	1:5:A:VAL:H	1:5:A:VAL:HG22	6	0.12
(3,14)	1:5:A:VAL:H	1:5:A:VAL:HG23	6	0.12
(2,744)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	7	0.12
(2,744)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	9	0.12
(2,737)	1:12:A:LEU:HB3	1:14:A:ASP:H	2	0.12
(2,720)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	2	0.12
(2,713)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	1	0.12
(2,713)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	1	0.12
(2,683)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	7	0.12
(2,683)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	7	0.12
(2,683)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	7	0.12
(2,675)	1:12:A:LEU:HB3	1:13:A:LYS:HD2	6	0.12
(2,671)	1:9:A:ILE:HD11	1:13:A:LYS:HE3	9	0.12
(2,671)	1:9:A:ILE:HD12	1:13:A:LYS:HE3	9	0.12
(2,671)	1:9:A:ILE:HD13	1:13:A:LYS:HE3	9	0.12
(2,647)	1:11:A:TRP:HA	1:21:A:ARG:HD3	5	0.12
(2,644)	1:8:A:TYR:HE1	1:11:A:TRP:HZ3	7	0.12
(2,644)	1:8:A:TYR:HE2	1:11:A:TRP:HZ3	7	0.12
(2,637)	1:8:A:TYR:HE1	1:25:A:CYS:HB3	6	0.12
(2,637)	1:8:A:TYR:HE2	1:25:A:CYS:HB3	6	0.12
(2,620)	1:16:A:GLY:H	1:19:A:SER:HB3	6	0.12
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	9	0.12
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	9	0.12
(2,550)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	9	0.12
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG21	9	0.12
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG22	9	0.12
(2,550)	1:8:A:TYR:HB3	1:9:A:ILE:HG23	9	0.12
(2,522)	1:3:A:GLU:HG2	1:4:A:CYS:HA	6	0.12
(2,522)	1:3:A:GLU:HG3	1:4:A:CYS:HA	6	0.12
(2,507)	1:11:A:TRP:HA	1:14:A:ASP:HB2	4	0.12
(2,507)	1:11:A:TRP:HA	1:14:A:ASP:HB2	10	0.12
(2,495)	1:5:A:VAL:HG11	1:6:A:ARG:HA	5	0.12
(2,495)	1:5:A:VAL:HG12	1:6:A:ARG:HA	5	0.12
(2,495)	1:5:A:VAL:HG13	1:6:A:ARG:HA	5	0.12
(2,495)	1:5:A:VAL:HG11	1:6:A:ARG:HA	10	0.12
(2,495)	1:5:A:VAL:HG12	1:6:A:ARG:HA	10	0.12
(2,495)	1:5:A:VAL:HG13	1:6:A:ARG:HA	10	0.12
(2,457)	1:11:A:TRP:HH2	1:17:A:PRO:HB3	3	0.12
(2,452)	1:11:A:TRP:HE3	1:23:A:PRO:HA	5	0.12
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	2	0.12
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	2	0.12
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	4	0.12
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	4	0.12
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	4	0.12
(2,402)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	10	0.12
(2,402)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	10	0.12
(2,362)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	9	0.12
(2,351)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	1	0.12
(2,351)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	6	0.12
(2,303)	1:17:A:PRO:HA	1:17:A:PRO:HD3	9	0.12
(2,273)	1:11:A:TRP:HE1	1:19:A:SER:HB3	4	0.12
(2,233)	1:9:A:ILE:H	1:9:A:ILE:HG13	10	0.12
(2,231)	1:7:A:LEU:H	1:7:A:LEU:HG	5	0.12
(2,192)	1:11:A:TRP:HE1	1:19:A:SER:HG	3	0.12
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB2	6	0.12
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB3	6	0.12
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB2	8	0.12
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB3	8	0.12
(2,166)	1:19:A:SER:H	1:19:A:SER:HB3	7	0.12
(2,152)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	5	0.12
(2,152)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	6	0.12
(2,146)	1:10:A:GLN:HA	1:10:A:GLN:HG3	2	0.12
(2,138)	1:18:A:SER:HA	1:18:A:SER:HB2	5	0.12
(2,131)	1:20:A:GLY:H	1:20:A:GLY:HA2	8	0.12
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG21	3	0.12
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG22	3	0.12
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG23	3	0.12
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG21	7	0.12
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG22	7	0.12
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG23	7	0.12
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG21	8	0.12
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG22	8	0.12
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG23	8	0.12
(2,92)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	6	0.12
(2,84)	1:14:A:ASP:H	1:14:A:ASP:HB2	1	0.12
(2,84)	1:14:A:ASP:H	1:14:A:ASP:HB2	7	0.12
(2,71)	1:5:A:VAL:H	1:5:A:VAL:HB	9	0.12
(2,61)	1:4:A:CYS:H	1:4:A:CYS:HB3	10	0.12
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD11	1	0.12
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD12	1	0.12
(1,724)	1:9:A:ILE:HB	1:9:A:ILE:HD13	1	0.12
(1,716)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	3	0.12
(1,716)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,716)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	3	0.12
(1,670)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	5	0.12
(1,670)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	5	0.12
(1,663)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	4	0.12
(1,514)	1:4:A:CYS:HA	1:7:A:LEU:HB2	7	0.12
(1,455)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	2	0.12
(1,447)	1:11:A:TRP:HD1	1:21:A:ARG:HG2	8	0.12
(1,447)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	8	0.12
(1,443)	1:23:A:PRO:HB2	1:25:A:CYS:H	2	0.12
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	2	0.12
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	2	0.12
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	2	0.12
(1,318)	1:17:A:PRO:HB2	1:17:A:PRO:HD3	7	0.12
(1,310)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	1	0.12
(1,310)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	3	0.12
(1,310)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	5	0.12
(1,310)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	7	0.12
(1,238)	1:6:A:ARG:HG2	1:7:A:LEU:H	8	0.12
(1,220)	1:21:A:ARG:HA	1:22:A:PRO:HD2	9	0.12
(1,193)	1:18:A:SER:H	1:19:A:SER:HB2	1	0.12
(1,193)	1:18:A:SER:H	1:19:A:SER:HB2	2	0.12
(1,187)	1:19:A:SER:H	1:19:A:SER:HG	10	0.12
(1,110)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	5	0.12
(1,73)	1:5:A:VAL:HB	1:6:A:ARG:H	1	0.12
(1,70)	1:10:A:GLN:H	1:10:A:GLN:HB3	4	0.12
(1,68)	1:10:A:GLN:H	1:10:A:GLN:HG3	1	0.12
(1,68)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.12
(1,35)	1:6:A:ARG:H	1:6:A:ARG:HG3	1	0.12
(1,31)	1:5:A:VAL:H	1:5:A:VAL:HG21	6	0.12
(1,31)	1:5:A:VAL:H	1:5:A:VAL:HG22	6	0.12
(1,31)	1:5:A:VAL:H	1:5:A:VAL:HG23	6	0.12
(1,15)	1:5:A:VAL:H	1:5:A:VAL:HG21	6	0.12
(1,15)	1:5:A:VAL:H	1:5:A:VAL:HG22	6	0.12
(1,15)	1:5:A:VAL:H	1:5:A:VAL:HG23	6	0.12
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	3	0.11
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	3	0.11
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	3	0.11
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	4	0.11
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	4	0.11
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	4	0.11
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	7	0.11
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	7	0.11
(3,620)	1:7:A:LEU:HD11	1:25:A:CYS:HA	9	0.11
(3,620)	1:7:A:LEU:HD12	1:25:A:CYS:HA	9	0.11
(3,620)	1:7:A:LEU:HD13	1:25:A:CYS:HA	9	0.11
(3,620)	1:7:A:LEU:HD21	1:25:A:CYS:HA	9	0.11
(3,620)	1:7:A:LEU:HD22	1:25:A:CYS:HA	9	0.11
(3,620)	1:7:A:LEU:HD23	1:25:A:CYS:HA	9	0.11
(3,597)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	3	0.11
(3,597)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	3	0.11
(3,597)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	6	0.11
(3,597)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	6	0.11
(3,597)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	10	0.11
(3,597)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	10	0.11
(3,584)	1:10:A:GLN:HA	1:13:A:LYS:H	2	0.11
(3,568)	1:11:A:TRP:HE1	1:17:A:PRO:HA	7	0.11
(3,545)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	7	0.11
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB2	8	0.11
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB3	8	0.11
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB2	10	0.11
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB3	10	0.11
(3,503)	1:7:A:LEU:HA	1:10:A:GLN:HB3	4	0.11
(3,503)	1:7:A:LEU:HA	1:10:A:GLN:HB3	10	0.11
(3,419)	1:8:A:TYR:HE1	1:12:A:LEU:HG	5	0.11
(3,419)	1:8:A:TYR:HE2	1:12:A:LEU:HG	5	0.11
(3,419)	1:8:A:TYR:HE1	1:12:A:LEU:HG	8	0.11
(3,419)	1:8:A:TYR:HE2	1:12:A:LEU:HG	8	0.11
(3,412)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.11
(3,225)	1:7:A:LEU:H	1:7:A:LEU:HB3	1	0.11
(3,222)	1:11:A:TRP:H	1:24:A:PRO:HG2	8	0.11
(3,212)	1:21:A:ARG:HA	1:22:A:PRO:HG2	7	0.11
(3,203)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	3	0.11
(3,203)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	6	0.11
(3,169)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	5	0.11
(3,169)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	5	0.11
(3,169)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	5	0.11
(3,169)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	7	0.11
(3,169)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	7	0.11
(3,169)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	7	0.11
(3,165)	1:19:A:SER:HA	1:19:A:SER:HB3	4	0.11
(3,93)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.11
(3,71)	1:5:A:VAL:HB	1:6:A:ARG:H	3	0.11
(3,33)	1:6:A:ARG:H	1:6:A:ARG:HG3	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:6:A:ARG:H	1:6:A:ARG:HG2	2	0.11
(3,25)	1:12:A:LEU:HD21	1:13:A:LYS:H	5	0.11
(3,25)	1:12:A:LEU:HD22	1:13:A:LYS:H	5	0.11
(3,25)	1:12:A:LEU:HD23	1:13:A:LYS:H	5	0.11
(3,25)	1:12:A:LEU:HD21	1:13:A:LYS:H	9	0.11
(3,25)	1:12:A:LEU:HD22	1:13:A:LYS:H	9	0.11
(3,25)	1:12:A:LEU:HD23	1:13:A:LYS:H	9	0.11
(3,10)	1:12:A:LEU:HD21	1:13:A:LYS:H	5	0.11
(3,10)	1:12:A:LEU:HD22	1:13:A:LYS:H	5	0.11
(3,10)	1:12:A:LEU:HD23	1:13:A:LYS:H	5	0.11
(3,10)	1:12:A:LEU:HD21	1:13:A:LYS:H	9	0.11
(3,10)	1:12:A:LEU:HD22	1:13:A:LYS:H	9	0.11
(3,10)	1:12:A:LEU:HD23	1:13:A:LYS:H	9	0.11
(2,680)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	3	0.11
(2,680)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	3	0.11
(2,680)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	3	0.11
(2,675)	1:12:A:LEU:HB3	1:13:A:LYS:HD2	3	0.11
(2,647)	1:11:A:TRP:HA	1:21:A:ARG:HD3	10	0.11
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	9	0.11
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	9	0.11
(2,522)	1:3:A:GLU:HG2	1:4:A:CYS:HA	1	0.11
(2,522)	1:3:A:GLU:HG3	1:4:A:CYS:HA	1	0.11
(2,511)	1:14:A:ASP:HB2	1:19:A:SER:HB2	6	0.11
(2,508)	1:14:A:ASP:HB3	1:19:A:SER:HA	10	0.11
(2,507)	1:11:A:TRP:HA	1:14:A:ASP:HB2	5	0.11
(2,495)	1:5:A:VAL:HG11	1:6:A:ARG:HA	9	0.11
(2,495)	1:5:A:VAL:HG12	1:6:A:ARG:HA	9	0.11
(2,495)	1:5:A:VAL:HG13	1:6:A:ARG:HA	9	0.11
(2,466)	1:17:A:PRO:HA	1:18:A:SER:H	9	0.11
(2,452)	1:11:A:TRP:HE3	1:23:A:PRO:HA	1	0.11
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	8	0.11
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	8	0.11
(2,411)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	8	0.11
(2,399)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	5	0.11
(2,394)	1:8:A:TYR:HE1	1:24:A:PRO:HD2	1	0.11
(2,394)	1:8:A:TYR:HE2	1:24:A:PRO:HD2	1	0.11
(2,394)	1:8:A:TYR:HE1	1:24:A:PRO:HD2	6	0.11
(2,394)	1:8:A:TYR:HE2	1:24:A:PRO:HD2	6	0.11
(2,306)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	1	0.11
(2,306)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	2	0.11
(2,306)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	3	0.11
(2,306)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,306)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	5	0.11
(2,306)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	6	0.11
(2,306)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	7	0.11
(2,306)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	8	0.11
(2,306)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	9	0.11
(2,306)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.11
(2,263)	1:9:A:ILE:HA	1:12:A:LEU:H	5	0.11
(2,263)	1:9:A:ILE:HA	1:12:A:LEU:H	9	0.11
(2,233)	1:9:A:ILE:H	1:9:A:ILE:HG13	2	0.11
(2,231)	1:7:A:LEU:H	1:7:A:LEU:HG	3	0.11
(2,184)	1:19:A:SER:HG	1:21:A:ARG:H	3	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB2	1	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB3	1	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB2	3	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB3	3	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB2	4	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB3	4	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB2	5	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB3	5	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB2	7	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB3	7	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB2	9	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB3	9	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB2	10	0.11
(2,171)	1:3:A:GLU:HA	1:3:A:GLU:HB3	10	0.11
(2,152)	1:10:A:GLN:HB2	1:10:A:GLN:HG2	7	0.11
(2,149)	1:10:A:GLN:HB3	1:10:A:GLN:HG2	5	0.11
(2,137)	1:18:A:SER:HA	1:18:A:SER:HB3	3	0.11
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG21	6	0.11
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG22	6	0.11
(2,124)	1:9:A:ILE:HA	1:9:A:ILE:HG23	6	0.11
(2,86)	1:14:A:ASP:HA	1:14:A:ASP:HB3	8	0.11
(2,84)	1:14:A:ASP:H	1:14:A:ASP:HB2	2	0.11
(2,84)	1:14:A:ASP:H	1:14:A:ASP:HB2	10	0.11
(2,71)	1:5:A:VAL:H	1:5:A:VAL:HB	2	0.11
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	3	0.11
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	3	0.11
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	3	0.11
(1,686)	1:7:A:LEU:HD11	1:25:A:CYS:HA	9	0.11
(1,686)	1:7:A:LEU:HD12	1:25:A:CYS:HA	9	0.11
(1,686)	1:7:A:LEU:HD13	1:25:A:CYS:HA	9	0.11
(1,686)	1:7:A:LEU:HD21	1:25:A:CYS:HA	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,686)	1:7:A:LEU:HD22	1:25:A:CYS:HA	9	0.11
(1,686)	1:7:A:LEU:HD23	1:25:A:CYS:HA	9	0.11
(1,659)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	3	0.11
(1,659)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	3	0.11
(1,659)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	6	0.11
(1,659)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	6	0.11
(1,659)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	10	0.11
(1,659)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	10	0.11
(1,646)	1:10:A:GLN:HA	1:13:A:LYS:H	2	0.11
(1,627)	1:11:A:TRP:HE1	1:17:A:PRO:HA	7	0.11
(1,601)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	7	0.11
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB2	8	0.11
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB3	8	0.11
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB2	10	0.11
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB3	10	0.11
(1,553)	1:7:A:LEU:HA	1:10:A:GLN:HB3	4	0.11
(1,553)	1:7:A:LEU:HA	1:10:A:GLN:HB3	10	0.11
(1,458)	1:8:A:TYR:HE1	1:12:A:LEU:HG	5	0.11
(1,458)	1:8:A:TYR:HE2	1:12:A:LEU:HG	5	0.11
(1,458)	1:8:A:TYR:HE1	1:12:A:LEU:HG	8	0.11
(1,458)	1:8:A:TYR:HE2	1:12:A:LEU:HG	8	0.11
(1,449)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.11
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	4	0.11
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	4	0.11
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	4	0.11
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	7	0.11
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	7	0.11
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	7	0.11
(1,236)	1:7:A:LEU:H	1:7:A:LEU:HB3	1	0.11
(1,232)	1:11:A:TRP:H	1:24:A:PRO:HG2	8	0.11
(1,222)	1:21:A:ARG:HA	1:22:A:PRO:HG2	7	0.11
(1,213)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	3	0.11
(1,213)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	6	0.11
(1,177)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	5	0.11
(1,177)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	5	0.11
(1,177)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	5	0.11
(1,177)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	7	0.11
(1,177)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	7	0.11
(1,177)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	7	0.11
(1,172)	1:19:A:SER:HA	1:19:A:SER:HB3	4	0.11
(1,98)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.11
(1,73)	1:5:A:VAL:HB	1:6:A:ARG:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:6:A:ARG:H	1:6:A:ARG:HG3	7	0.11
(1,34)	1:6:A:ARG:H	1:6:A:ARG:HG2	2	0.11
(1,27)	1:12:A:LEU:HD21	1:13:A:LYS:H	5	0.11
(1,27)	1:12:A:LEU:HD22	1:13:A:LYS:H	5	0.11
(1,27)	1:12:A:LEU:HD23	1:13:A:LYS:H	5	0.11
(1,27)	1:12:A:LEU:HD21	1:13:A:LYS:H	9	0.11
(1,27)	1:12:A:LEU:HD22	1:13:A:LYS:H	9	0.11
(1,27)	1:12:A:LEU:HD23	1:13:A:LYS:H	9	0.11
(1,11)	1:12:A:LEU:HD21	1:13:A:LYS:H	5	0.11
(1,11)	1:12:A:LEU:HD22	1:13:A:LYS:H	5	0.11
(1,11)	1:12:A:LEU:HD23	1:13:A:LYS:H	5	0.11
(1,11)	1:12:A:LEU:HD21	1:13:A:LYS:H	9	0.11
(1,11)	1:12:A:LEU:HD22	1:13:A:LYS:H	9	0.11
(1,11)	1:12:A:LEU:HD23	1:13:A:LYS:H	9	0.11
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	2	0.1
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	2	0.1
(4,70)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	2	0.1
(4,45)	1:4:A:CYS:HA	1:7:A:LEU:HB2	10	0.1
(4,37)	1:23:A:PRO:HB2	1:25:A:CYS:H	9	0.1
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	8	0.1
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	8	0.1
(4,31)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	8	0.1
(3,621)	1:6:A:ARG:HA	1:9:A:ILE:HD11	6	0.1
(3,621)	1:6:A:ARG:HA	1:9:A:ILE:HD12	6	0.1
(3,621)	1:6:A:ARG:HA	1:9:A:ILE:HD13	6	0.1
(3,620)	1:7:A:LEU:HD11	1:25:A:CYS:HA	2	0.1
(3,620)	1:7:A:LEU:HD12	1:25:A:CYS:HA	2	0.1
(3,620)	1:7:A:LEU:HD13	1:25:A:CYS:HA	2	0.1
(3,620)	1:7:A:LEU:HD21	1:25:A:CYS:HA	2	0.1
(3,620)	1:7:A:LEU:HD22	1:25:A:CYS:HA	2	0.1
(3,620)	1:7:A:LEU:HD23	1:25:A:CYS:HA	2	0.1
(3,620)	1:7:A:LEU:HD11	1:25:A:CYS:HA	5	0.1
(3,620)	1:7:A:LEU:HD12	1:25:A:CYS:HA	5	0.1
(3,620)	1:7:A:LEU:HD13	1:25:A:CYS:HA	5	0.1
(3,620)	1:7:A:LEU:HD21	1:25:A:CYS:HA	5	0.1
(3,620)	1:7:A:LEU:HD22	1:25:A:CYS:HA	5	0.1
(3,620)	1:7:A:LEU:HD23	1:25:A:CYS:HA	5	0.1
(3,614)	1:3:A:GLU:HA	1:6:A:ARG:HB3	1	0.1
(3,597)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	9	0.1
(3,597)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	9	0.1
(3,590)	1:17:A:PRO:HD3	1:18:A:SER:H	7	0.1
(3,565)	1:8:A:TYR:HB2	1:12:A:LEU:H	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,565)	1:8:A:TYR:HB3	1:12:A:LEU:H	5	0.1
(3,565)	1:8:A:TYR:HB2	1:12:A:LEU:H	9	0.1
(3,565)	1:8:A:TYR:HB3	1:12:A:LEU:H	9	0.1
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB2	1	0.1
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB3	1	0.1
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB2	9	0.1
(3,505)	1:2:A:GLU:HA	1:3:A:GLU:HB3	9	0.1
(3,472)	1:8:A:TYR:HA	1:11:A:TRP:HB2	8	0.1
(3,412)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	1	0.1
(3,362)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.1
(3,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	4	0.1
(3,289)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	2	0.1
(3,232)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.1
(3,222)	1:11:A:TRP:H	1:24:A:PRO:HG2	1	0.1
(3,222)	1:11:A:TRP:H	1:24:A:PRO:HG2	3	0.1
(3,203)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.1
(3,203)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	9	0.1
(3,169)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	10	0.1
(3,169)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	10	0.1
(3,169)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	10	0.1
(3,71)	1:5:A:VAL:HB	1:6:A:ARG:H	2	0.1
(3,65)	1:10:A:GLN:H	1:10:A:GLN:HG2	2	0.1
(3,25)	1:12:A:LEU:HD21	1:13:A:LYS:H	3	0.1
(3,25)	1:12:A:LEU:HD22	1:13:A:LYS:H	3	0.1
(3,25)	1:12:A:LEU:HD23	1:13:A:LYS:H	3	0.1
(3,10)	1:12:A:LEU:HD21	1:13:A:LYS:H	3	0.1
(3,10)	1:12:A:LEU:HD22	1:13:A:LYS:H	3	0.1
(3,10)	1:12:A:LEU:HD23	1:13:A:LYS:H	3	0.1
(2,742)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	4	0.1
(2,742)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	8	0.1
(2,706)	1:7:A:LEU:HG	1:25:A:CYS:HB2	1	0.1
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	6	0.1
(2,531)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	6	0.1
(2,495)	1:5:A:VAL:HG11	1:6:A:ARG:HA	1	0.1
(2,495)	1:5:A:VAL:HG12	1:6:A:ARG:HA	1	0.1
(2,495)	1:5:A:VAL:HG13	1:6:A:ARG:HA	1	0.1
(2,452)	1:11:A:TRP:HE3	1:23:A:PRO:HA	7	0.1
(2,425)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	4	0.1
(2,425)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	4	0.1
(2,382)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.1
(2,367)	1:8:A:TYR:HA	1:8:A:TYR:HD1	4	0.1
(2,367)	1:8:A:TYR:HA	1:8:A:TYR:HD2	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,298)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	1	0.1
(2,298)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	1	0.1
(2,298)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	1	0.1
(2,298)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	1	0.1
(2,298)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	1	0.1
(2,298)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	1	0.1
(2,298)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	1	0.1
(2,298)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	1	0.1
(2,298)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	1	0.1
(2,185)	1:20:A:GLY:HA3	1:21:A:ARG:H	5	0.1
(2,149)	1:10:A:GLN:HB3	1:10:A:GLN:HG2	6	0.1
(2,127)	1:9:A:ILE:HB	1:9:A:ILE:HG21	7	0.1
(2,127)	1:9:A:ILE:HB	1:9:A:ILE:HG22	7	0.1
(2,127)	1:9:A:ILE:HB	1:9:A:ILE:HG23	7	0.1
(2,127)	1:9:A:ILE:HB	1:9:A:ILE:HG21	8	0.1
(2,127)	1:9:A:ILE:HB	1:9:A:ILE:HG22	8	0.1
(2,127)	1:9:A:ILE:HB	1:9:A:ILE:HG23	8	0.1
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	2	0.1
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	2	0.1
(1,717)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	2	0.1
(1,687)	1:6:A:ARG:HA	1:9:A:ILE:HD11	6	0.1
(1,687)	1:6:A:ARG:HA	1:9:A:ILE:HD12	6	0.1
(1,687)	1:6:A:ARG:HA	1:9:A:ILE:HD13	6	0.1
(1,686)	1:7:A:LEU:HD11	1:25:A:CYS:HA	2	0.1
(1,686)	1:7:A:LEU:HD12	1:25:A:CYS:HA	2	0.1
(1,686)	1:7:A:LEU:HD13	1:25:A:CYS:HA	2	0.1
(1,686)	1:7:A:LEU:HD21	1:25:A:CYS:HA	2	0.1
(1,686)	1:7:A:LEU:HD22	1:25:A:CYS:HA	2	0.1
(1,686)	1:7:A:LEU:HD23	1:25:A:CYS:HA	2	0.1
(1,686)	1:7:A:LEU:HD11	1:25:A:CYS:HA	5	0.1
(1,686)	1:7:A:LEU:HD12	1:25:A:CYS:HA	5	0.1
(1,686)	1:7:A:LEU:HD13	1:25:A:CYS:HA	5	0.1
(1,686)	1:7:A:LEU:HD21	1:25:A:CYS:HA	5	0.1
(1,686)	1:7:A:LEU:HD22	1:25:A:CYS:HA	5	0.1
(1,686)	1:7:A:LEU:HD23	1:25:A:CYS:HA	5	0.1
(1,679)	1:3:A:GLU:HA	1:6:A:ARG:HB3	1	0.1
(1,659)	1:8:A:TYR:HD1	1:24:A:PRO:HB2	9	0.1
(1,659)	1:8:A:TYR:HD2	1:24:A:PRO:HB2	9	0.1
(1,652)	1:17:A:PRO:HD3	1:18:A:SER:H	7	0.1
(1,624)	1:8:A:TYR:HB2	1:12:A:LEU:H	5	0.1
(1,624)	1:8:A:TYR:HB3	1:12:A:LEU:H	5	0.1
(1,624)	1:8:A:TYR:HB2	1:12:A:LEU:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:8:A:TYR:HB3	1:12:A:LEU:H	9	0.1
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB2	1	0.1
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB3	1	0.1
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB2	9	0.1
(1,555)	1:2:A:GLU:HA	1:3:A:GLU:HB3	9	0.1
(1,519)	1:8:A:TYR:HA	1:11:A:TRP:HB2	8	0.1
(1,514)	1:4:A:CYS:HA	1:7:A:LEU:HB2	10	0.1
(1,449)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	1	0.1
(1,443)	1:23:A:PRO:HB2	1:25:A:CYS:H	9	0.1
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	8	0.1
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	8	0.1
(1,425)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	8	0.1
(1,386)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.1
(1,368)	1:24:A:PRO:HB2	1:24:A:PRO:HG3	4	0.1
(1,310)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	2	0.1
(1,244)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.1
(1,232)	1:11:A:TRP:H	1:24:A:PRO:HG2	1	0.1
(1,232)	1:11:A:TRP:H	1:24:A:PRO:HG2	3	0.1
(1,213)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.1
(1,213)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	9	0.1
(1,177)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	10	0.1
(1,177)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	10	0.1
(1,177)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	10	0.1
(1,73)	1:5:A:VAL:HB	1:6:A:ARG:H	2	0.1
(1,67)	1:10:A:GLN:H	1:10:A:GLN:HG2	2	0.1
(1,27)	1:12:A:LEU:HD21	1:13:A:LYS:H	3	0.1
(1,27)	1:12:A:LEU:HD22	1:13:A:LYS:H	3	0.1
(1,27)	1:12:A:LEU:HD23	1:13:A:LYS:H	3	0.1
(1,11)	1:12:A:LEU:HD21	1:13:A:LYS:H	3	0.1
(1,11)	1:12:A:LEU:HD22	1:13:A:LYS:H	3	0.1
(1,11)	1:12:A:LEU:HD23	1:13:A:LYS:H	3	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found