



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 12:46 PM UTC

PDB ID : 9GE1 / pdb_00009ge1
BMRB ID : 34949
Title : Trp-cage fortified Tc5b-Exenatide chimera with disulfide bond cyclization (Ex-4-Tc5bCC) at 321K
Authors : Horvath, D.
Deposited on : 2024-08-06

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 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

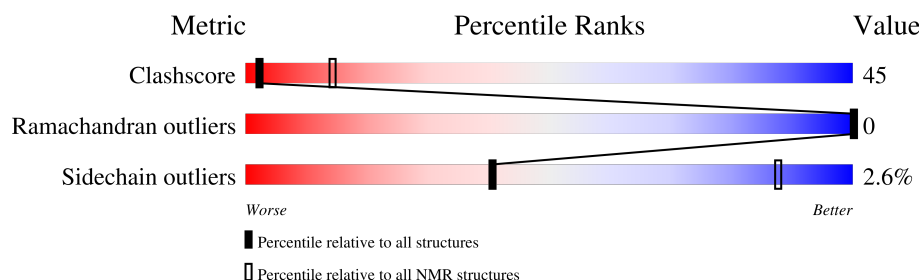
1 Overall quality at a glance

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	52% 36% 12%

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:4-A:25 (22)	0.25	5

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

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

The models can be grouped into 2 clusters and 5 single-model clusters were found.

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

3 Entry composition [i](#)

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

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

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

4 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-Tc5bCC)

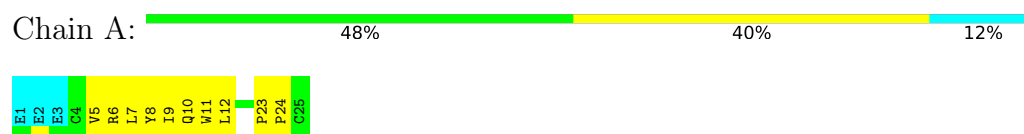


4.2 Scores per residue for each member of the ensemble

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-Tc5bCC)



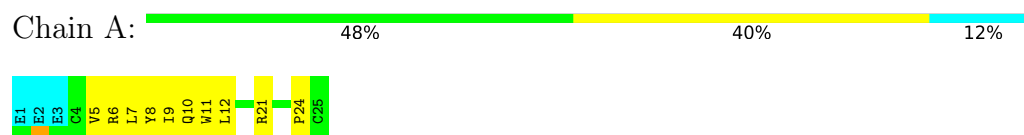
4.2.2 Score per residue for model 2

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



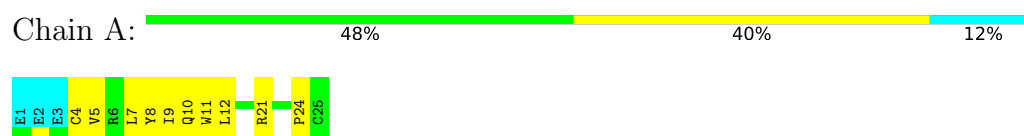
4.2.3 Score per residue for model 3

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



4.2.4 Score per residue for model 4

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



4.2.5 Score per residue for model 5 (medoid)

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



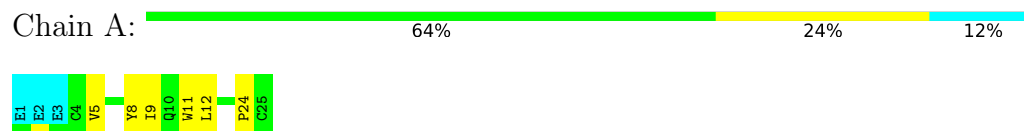
4.2.6 Score per residue for model 6

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



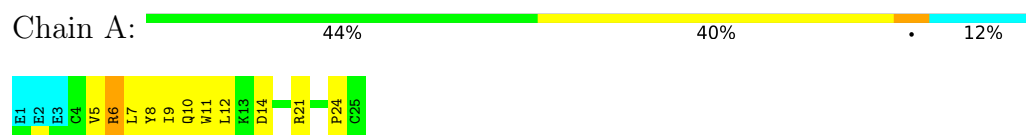
4.2.7 Score per residue for model 7

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



4.2.8 Score per residue for model 8

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



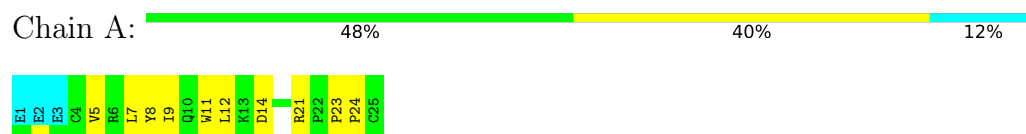
4.2.9 Score per residue for model 9

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



4.2.10 Score per residue for model 10

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



5 Refinement protocol and experimental data overview

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

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

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

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

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	165
Number of shifts mapped to atoms	165
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

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	170	167	167	15±2
All	All	1700	1670	1670	153

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 45.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:TRP:CE3	1:A:12:LEU:HD22	0.65	2.27	1	10
1:A:8:TYR:O	1:A:11:TRP:HB3	0.64	1.92	6	10
1:A:8:TYR:C	1:A:12:LEU:HD23	0.57	2.24	6	10
1:A:8:TYR:HA	1:A:24:PRO:CG	0.57	2.29	1	10
1:A:11:TRP:HE3	1:A:12:LEU:HD22	0.56	1.59	9	10
1:A:11:TRP:CH2	1:A:23:PRO:HG3	0.56	2.35	1	2
1:A:9:ILE:HA	1:A:12:LEU:HB2	0.54	1.80	4	10
1:A:8:TYR:O	1:A:12:LEU:HD23	0.54	2.03	4	10
1:A:7:LEU:O	1:A:24:PRO:HG3	0.50	2.06	4	2
1:A:5:VAL:HG12	1:A:9:ILE:HD12	0.50	1.83	6	8
1:A:7:LEU:C	1:A:24:PRO:HG3	0.50	2.32	4	8
1:A:11:TRP:CD1	1:A:21:ARG:HB3	0.50	2.42	3	4
1:A:5:VAL:O	1:A:8:TYR:HB3	0.49	2.07	4	7
1:A:9:ILE:HA	1:A:12:LEU:HD23	0.49	1.83	2	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:TRP:CZ2	1:A:23:PRO:HG3	0.48	2.43	1	2
1:A:7:LEU:O	1:A:10:GLN:HB3	0.46	2.10	2	6
1:A:8:TYR:CE2	1:A:12:LEU:HD21	0.46	2.46	2	2
1:A:8:TYR:O	1:A:11:TRP:N	0.46	2.49	2	10
1:A:8:TYR:HA	1:A:24:PRO:HG2	0.46	1.86	7	1
1:A:11:TRP:HE3	1:A:12:LEU:CD2	0.45	2.24	10	10
1:A:5:VAL:HA	1:A:8:TYR:HB3	0.44	1.88	8	2
1:A:8:TYR:CE1	1:A:12:LEU:HD21	0.43	2.47	1	2
1:A:11:TRP:CE3	1:A:12:LEU:CD2	0.43	3.02	3	5
1:A:12:LEU:HD22	1:A:12:LEU:N	0.41	2.30	10	2
1:A:9:ILE:CA	1:A:12:LEU:HD23	0.41	2.45	2	1
1:A:12:LEU:CD2	1:A:12:LEU:N	0.41	2.84	4	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	21/25 (84%)	19±1 (90±4%)	2±1 (10±4%)	0±0 (0±0%)	100	100
All	All	210/250 (84%)	188 (90%)	22 (10%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	19/22 (86%)	18±1 (97±4%)	0±1 (3±4%)	41	88
All	All	190/220 (86%)	185 (97%)	5 (3%)	41	88

All 3 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	6	ARG	2
1	A	14	ASP	2
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 [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 51% for the well-defined parts and 50% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *nef_chemical_shift_list_ShiftList_1*

7.1.1 Bookkeeping

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	165
Number of shifts mapped to atoms	165
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

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 51%, i.e. 149 atoms were assigned a chemical shift out of a possible 292. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	42/105 (40%)	42/43 (98%)	0/44 (0%)	0/18 (0%)
Sidechain	97/166 (58%)	97/108 (90%)	0/50 (0%)	0/8 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	149/292 (51%)	149/161 (93%)	0/104 (0%)	0/27 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 165 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	46/120 (38%)	46/49 (94%)	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	165/328 (50%)	165/179 (92%)	0/119 (0%)	0/30 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

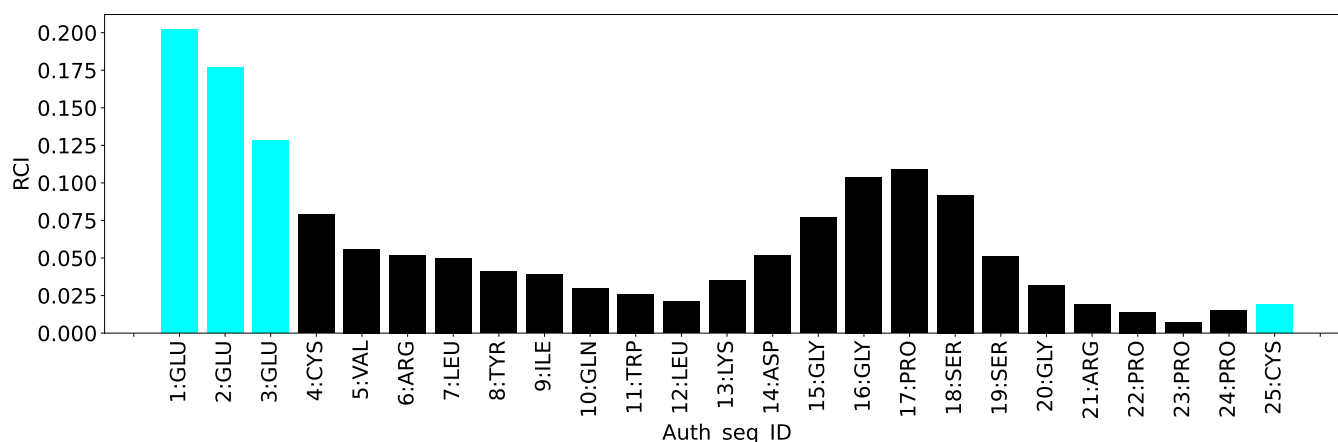
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	16	GLY	HA2	0.83	2.15 – 5.77	-8.7
1	A	23	PRO	HA	2.33	2.78 – 6.00	-6.4

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	1866
Intra-residue ($ i-j =0$)	921
Sequential ($ i-j =1$)	336
Medium range ($ i-j >1$ and $ i-j <5$)	336
Long range ($ i-j \geq 5$)	273
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	74.6
Number of long range restraints per residue ¹	10.9

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)	71.2	0.2
0.2-0.5 (Medium)	157.1	0.5
>0.5 (Large)	133.5	2.57

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

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

9 Distance violation analysis ⓘ

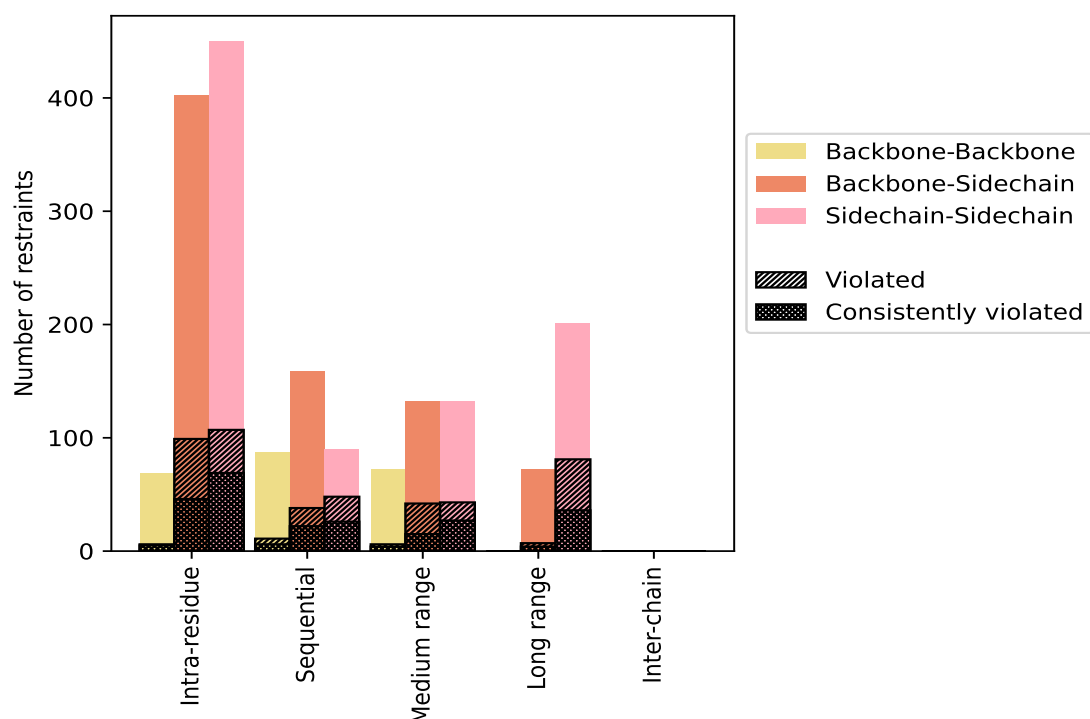
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	921	49.4	212	23.0	11.4	120	13.0	6.4
Backbone-Backbone	69	3.7	6	8.7	0.3	5	7.2	0.3
Backbone-Sidechain	402	21.5	99	24.6	5.3	46	11.4	2.5
Sidechain-Sidechain	450	24.1	107	23.8	5.7	69	15.3	3.7
Sequential (i-j =1)	336	18.0	97	28.9	5.2	54	16.1	2.9
Backbone-Backbone	87	4.7	11	12.6	0.6	6	6.9	0.3
Backbone-Sidechain	159	8.5	38	23.9	2.0	22	13.8	1.2
Sidechain-Sidechain	90	4.8	48	53.3	2.6	26	28.9	1.4
Medium range (i-j >1 & i-j <5)	336	18.0	91	27.1	4.9	46	13.7	2.5
Backbone-Backbone	72	3.9	6	8.3	0.3	4	5.6	0.2
Backbone-Sidechain	132	7.1	42	31.8	2.3	15	11.4	0.8
Sidechain-Sidechain	132	7.1	43	32.6	2.3	27	20.5	1.4
Long range (i-j ≥5)	273	14.6	88	32.2	4.7	40	14.7	2.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	72	3.9	7	9.7	0.4	4	5.6	0.2
Sidechain-Sidechain	201	10.8	81	40.3	4.3	36	17.9	1.9
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	1866	100.0	488	26.2	26.2	260	13.9	13.9
Backbone-Backbone	228	12.2	23	10.1	1.2	15	6.6	0.8
Backbone-Sidechain	765	41.0	186	24.3	10.0	87	11.4	4.7
Sidechain-Sidechain	873	46.8	279	32.0	15.0	158	18.1	8.5

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

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



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

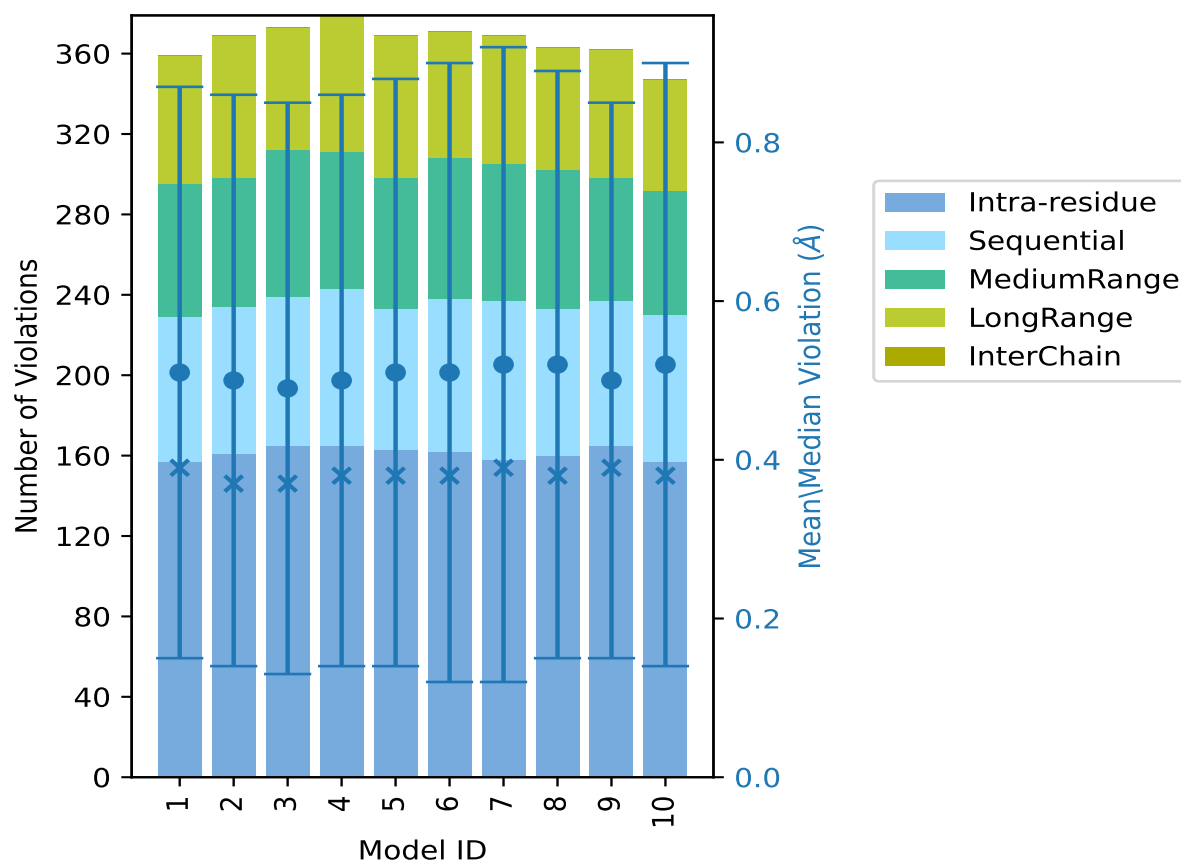
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	157	72	66	64	0	359	0.51	1.81	0.36	0.39
2	161	73	64	71	0	369	0.5	1.91	0.36	0.37
3	165	74	73	61	0	373	0.49	1.86	0.36	0.37
4	165	78	68	68	0	379	0.5	1.67	0.36	0.38
5	163	70	65	71	0	369	0.51	2.03	0.37	0.38
6	162	76	70	63	0	371	0.51	2.55	0.39	0.38
7	158	79	68	64	0	369	0.52	2.57	0.4	0.39
8	160	73	69	61	0	363	0.52	2.29	0.37	0.38
9	165	72	61	64	0	362	0.5	1.73	0.35	0.39
10	157	73	62	55	0	347	0.52	2.35	0.38	0.38

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, 1378(IR:709, SQ:239, MR:245, LR:185, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
13	9	7	4	0	33	1	10.0
16	6	8	8	0	38	2	20.0
13	6	6	4	0	29	3	30.0

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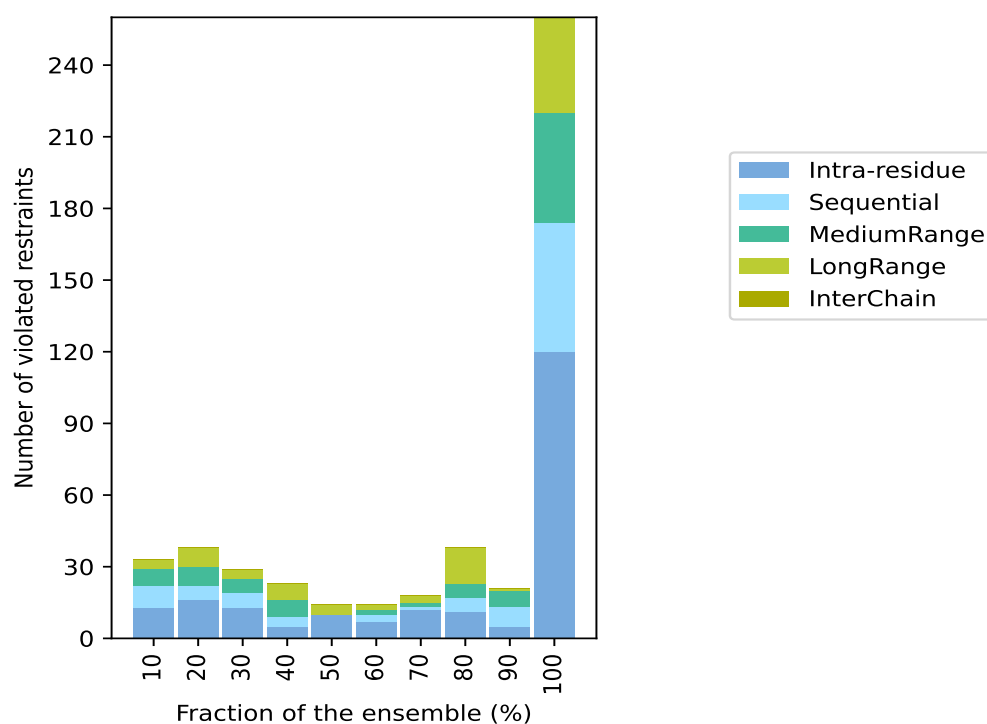
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
5	4	7	7	0	23	4	40.0
10	0	0	4	0	14	5	50.0
7	3	2	2	0	14	6	60.0
12	1	2	3	0	18	7	70.0
11	6	6	15	0	38	8	80.0
5	8	7	1	0	21	9	90.0
120	54	46	40	0	260	10	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](#)

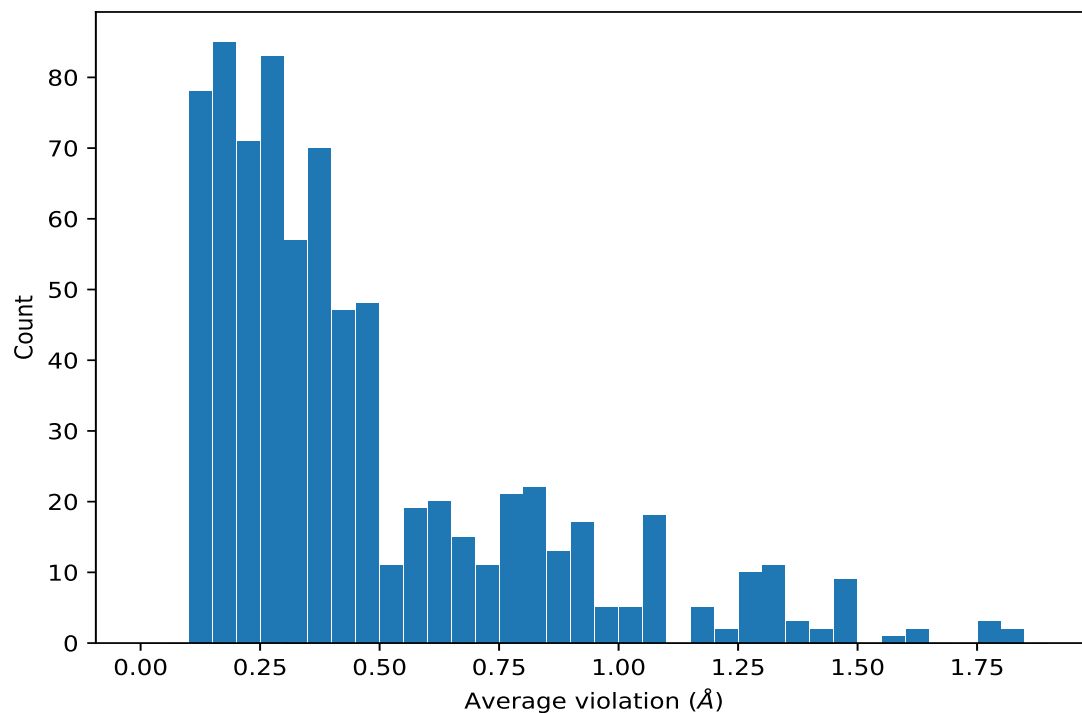


9.4 Most violated distance restraints in the ensemble [i](#)

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)
(2,88)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.84	0.12	1.86
(4,5)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.84	0.12	1.86
(1,520)	1:1:A:GLU:HA	1:1:A:GLU:HG2	10	1.79	0.34	1.76
(2,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	1.77	0.4	1.58
(4,29)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	1.77	0.4	1.58
(1,563)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	10	1.62	0.04	1.62
(1,563)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	10	1.62	0.04	1.62
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	10	1.47	0.01	1.46
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	10	1.47	0.01	1.46
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	10	1.47	0.01	1.46
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	10	1.46	0.01	1.46
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	10	1.46	0.01	1.46
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	10	1.46	0.01	1.46
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	10	1.46	0.01	1.46
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	10	1.46	0.01	1.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	10	1.46	0.01	1.46
(2,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.4	0.01	1.4
(3,129)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.4	0.01	1.4
(1,549)	1:20:A:GLY:H	1:21:A:ARG:H	10	1.39	0.12	1.35
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	10	1.31	0.06	1.33
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	10	1.31	0.06	1.33
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	10	1.31	0.06	1.33
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	10	1.31	0.06	1.33
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	10	1.31	0.06	1.33
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	10	1.31	0.06	1.33
(1,394)	1:22:A:PRO:HA	1:22:A:PRO:HD3	10	1.31	0.05	1.33
(2,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	1.31	0.08	1.34
(3,124)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	1.31	0.08	1.34
(2,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	10	1.3	0.17	1.31
(3,454)	1:4:A:CYS:HA	1:7:A:LEU:HB3	10	1.3	0.17	1.31
(2,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	1.25	0.03	1.25
(2,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	1.25	0.03	1.25
(3,140)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	1.25	0.03	1.25
(3,140)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	1.25	0.03	1.25
(1,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	1.23	0.4	1.04
(1,88)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.23	0.12	1.25
(1,466)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	1.17	0.22	1.27
(1,190)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	10	1.16	0.02	1.17
(1,190)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	10	1.16	0.02	1.17
(2,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	1.16	0.03	1.16
(4,18)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	1.16	0.03	1.16
(2,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	10	1.08	0.03	1.09
(2,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	10	1.08	0.03	1.09
(2,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	10	1.08	0.03	1.09
(3,552)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	10	1.08	0.03	1.09
(3,552)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	10	1.08	0.03	1.09
(3,552)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	10	1.08	0.03	1.09
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	1.05	0.03	1.04
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	1.05	0.03	1.04
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	1.05	0.03	1.04
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	1.05	0.03	1.04
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	1.05	0.03	1.04
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	1.05	0.03	1.04
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	1.05	0.03	1.04
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	1.05	0.03	1.04
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	1.05	0.03	1.04
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	1.05	0.03	1.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	1.05	0.03	1.04
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	1.05	0.03	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD21	10	1.03	0.02	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD22	10	1.03	0.02	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD23	10	1.03	0.02	1.04
(1,487)	1:8:A:TYR:HA	1:24:A:PRO:HD2	10	1.02	0.08	1.04
(1,342)	1:13:A:LYS:HA	1:13:A:LYS:HD2	10	1.0	0.12	1.0
(1,362)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	10	0.98	0.24	1.1
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG2	10	0.95	0.03	0.95
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG3	10	0.95	0.03	0.95
(1,609)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	10	0.94	0.07	0.95
(1,609)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	10	0.94	0.07	0.95
(1,609)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	10	0.94	0.07	0.95
(1,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	0.93	0.01	0.93
(2,97)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.92	0.02	0.93
(4,7)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.92	0.02	0.93
(1,490)	1:14:A:ASP:HB3	1:19:A:SER:HB2	10	0.92	0.4	1.1
(1,521)	1:1:A:GLU:HA	1:1:A:GLU:HG3	10	0.92	0.58	0.8
(1,473)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	10	0.91	0.15	0.95
(1,423)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	10	0.91	0.09	0.93
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD21	10	0.9	0.03	0.9
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD22	10	0.9	0.03	0.9
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD23	10	0.9	0.03	0.9
(1,519)	1:1:A:GLU:HA	1:1:A:GLU:HB3	10	0.9	0.23	0.98
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG2	10	0.89	0.08	0.85
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG3	10	0.89	0.08	0.85
(2,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.88	0.01	0.88
(3,138)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.88	0.01	0.88
(1,476)	1:9:A:ILE:HA	1:12:A:LEU:HG	10	0.86	0.06	0.88
(1,480)	1:8:A:TYR:HA	1:24:A:PRO:HG3	10	0.85	0.1	0.88
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD21	10	0.85	0.03	0.84
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD22	10	0.85	0.03	0.84
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD23	10	0.85	0.03	0.84
(2,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	10	0.85	0.08	0.82
(3,444)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	10	0.85	0.08	0.82
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	10	0.82	0.09	0.86
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	10	0.82	0.09	0.86
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	10	0.82	0.09	0.86
(2,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.82	0.0	0.82
(3,132)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.82	0.0	0.82
(1,605)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	10	0.82	0.03	0.83
(1,605)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	10	0.82	0.03	0.83

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,605)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	10	0.82	0.03	0.83
(2,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	10	0.8	0.03	0.8
(2,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	10	0.8	0.03	0.8
(3,139)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	10	0.8	0.03	0.8
(3,139)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	10	0.8	0.03	0.8
(1,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	10	0.79	0.03	0.8
(1,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	10	0.79	0.03	0.8
(1,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	10	0.79	0.03	0.8
(2,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.79	0.03	0.8
(3,43)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.79	0.03	0.8
(2,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.78	0.09	0.78
(3,142)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.78	0.09	0.78
(1,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.78	0.03	0.78
(1,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.78	0.03	0.78
(2,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.78	0.01	0.78
(3,417)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.78	0.01	0.78
(1,398)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.77	0.02	0.78
(2,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.76	0.06	0.77
(2,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.76	0.06	0.77
(2,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.76	0.06	0.77
(3,578)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.76	0.06	0.77
(3,578)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.76	0.06	0.77
(3,578)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.76	0.06	0.77
(1,397)	1:22:A:PRO:HA	1:22:A:PRO:HG3	10	0.75	0.23	0.72
(1,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	0.74	0.08	0.78
(2,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.74	0.03	0.74
(4,31)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.74	0.03	0.74
(1,322)	1:11:A:TRP:HA	1:11:A:TRP:HB2	10	0.73	0.01	0.74
(1,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	10	0.72	0.17	0.73
(1,575)	1:2:A:GLU:HB2	1:6:A:ARG:HA	10	0.71	0.17	0.66
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	10	0.71	0.01	0.71
(3,86)	1:7:A:LEU:H	1:7:A:LEU:HB3	10	0.71	0.01	0.71
(1,101)	1:24:A:PRO:HG2	1:25:A:CYS:H	10	0.69	0.14	0.7
(1,360)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.68	0.03	0.67
(1,199)	1:24:A:PRO:HD2	1:25:A:CYS:H	10	0.68	0.09	0.72
(1,437)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.67	0.01	0.68
(1,494)	1:22:A:PRO:HA	1:23:A:PRO:HD2	10	0.67	0.07	0.7
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	10	0.67	0.1	0.62
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	10	0.67	0.1	0.62
(2,96)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.67	0.01	0.67
(3,90)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.67	0.01	0.67
(1,299)	1:9:A:ILE:HA	1:9:A:ILE:HG12	10	0.65	0.02	0.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,145)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.64	0.01	0.64
(3,135)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.64	0.01	0.64
(2,562)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	10	0.64	0.07	0.65
(3,530)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	10	0.64	0.07	0.65
(2,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.63	0.16	0.58
(3,125)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.63	0.16	0.58
(2,305)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.62	0.0	0.62
(3,279)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.62	0.0	0.62
(1,418)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.62	0.01	0.62
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG2	10	0.62	0.03	0.62
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG3	10	0.62	0.03	0.62
(1,393)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.6	0.05	0.6
(2,620)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	10	0.6	0.03	0.6
(4,38)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	10	0.6	0.03	0.6
(1,415)	1:21:A:ARG:HA	1:22:A:PRO:HD3	10	0.59	0.05	0.62
(1,354)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.59	0.0	0.59
(1,612)	1:9:A:ILE:HG21	1:12:A:LEU:HB2	10	0.58	0.05	0.58
(1,612)	1:9:A:ILE:HG22	1:12:A:LEU:HB2	10	0.58	0.05	0.58
(1,612)	1:9:A:ILE:HG23	1:12:A:LEU:HB2	10	0.58	0.05	0.58
(1,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.57	0.01	0.57
(1,119)	1:8:A:TYR:HB3	1:9:A:ILE:H	10	0.57	0.01	0.57
(2,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.57	0.17	0.57
(3,141)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.57	0.17	0.57
(1,224)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	10	0.56	0.05	0.58
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB2	10	0.55	0.04	0.55
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB3	10	0.55	0.04	0.55
(1,529)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	10	0.55	0.3	0.46
(1,456)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	10	0.55	0.16	0.62
(1,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.54	0.03	0.56
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG2	10	0.54	0.03	0.54
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG3	10	0.54	0.03	0.54
(1,53)	1:18:A:SER:H	1:18:A:SER:HB2	10	0.54	0.08	0.58
(1,181)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.54	0.18	0.46
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	10	0.49	0.05	0.5
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	10	0.49	0.05	0.5
(1,443)	1:24:A:PRO:HA	1:24:A:PRO:HD3	10	0.48	0.04	0.47
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.48	0.02	0.49
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.48	0.02	0.49
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.48	0.02	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.48	0.02	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.48	0.02	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.48	0.02	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	10	0.48	0.05	0.48
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG3	10	0.48	0.05	0.48
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	10	0.48	0.05	0.48
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG3	10	0.48	0.05	0.48
(1,149)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	10	0.47	0.02	0.48
(1,149)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	10	0.47	0.02	0.48
(1,510)	1:12:A:LEU:HA	1:16:A:GLY:HA3	10	0.47	0.08	0.48
(1,278)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.46	0.05	0.47
(2,598)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	10	0.46	0.04	0.46
(2,598)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	10	0.46	0.04	0.46
(2,598)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	10	0.46	0.04	0.46
(3,564)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	10	0.46	0.04	0.46
(3,564)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	10	0.46	0.04	0.46
(3,564)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	10	0.46	0.04	0.46
(1,146)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	0.45	0.01	0.45
(1,286)	1:7:A:LEU:HA	1:7:A:LEU:HB3	10	0.45	0.03	0.44
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	0.45	0.03	0.44
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	0.45	0.03	0.44
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	0.45	0.03	0.44
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	0.45	0.03	0.44
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	0.45	0.03	0.44
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	0.45	0.03	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.44	0.0	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.44	0.0	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.44	0.0	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	10	0.44	0.0	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	10	0.44	0.0	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	10	0.44	0.0	0.44
(2,340)	1:12:A:LEU:HB3	1:13:A:LYS:H	10	0.44	0.03	0.46
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	10	0.44	0.03	0.46
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	10	0.44	0.01	0.44
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	10	0.44	0.01	0.44
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	10	0.44	0.01	0.44
(1,1)	1:7:A:LEU:HB2	1:8:A:TYR:H	10	0.44	0.04	0.45
(1,352)	1:14:A:ASP:HA	1:14:A:ASP:HB2	10	0.44	0.06	0.42
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD11	10	0.43	0.04	0.42
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD12	10	0.43	0.04	0.42
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD13	10	0.43	0.04	0.42
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD11	10	0.43	0.04	0.42
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD12	10	0.43	0.04	0.42
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD13	10	0.43	0.04	0.42
(1,406)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.42	0.02	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	0.42	0.01	0.42
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	0.42	0.01	0.42
(1,438)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	10	0.41	0.07	0.44
(1,404)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.4	0.02	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.4	0.0	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	10	0.4	0.0	0.4
(1,94)	1:9:A:ILE:H	1:9:A:ILE:HG13	10	0.4	0.03	0.39
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.39	0.12	0.42
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	10	0.39	0.12	0.42
(2,232)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.39	0.03	0.37
(2,232)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.39	0.03	0.37
(2,232)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.39	0.03	0.37
(4,22)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.39	0.03	0.37
(4,22)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.39	0.03	0.37
(4,22)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.39	0.03	0.37
(1,429)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.39	0.02	0.38
(1,113)	1:9:A:ILE:HA	1:12:A:LEU:H	10	0.38	0.05	0.38
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	10	0.38	0.06	0.38
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	10	0.38	0.06	0.38
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	10	0.38	0.06	0.38
(1,526)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	10	0.38	0.0	0.38
(2,233)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.38	0.03	0.38
(2,233)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.38	0.03	0.38
(2,233)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.38	0.03	0.38
(4,23)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.38	0.03	0.38
(4,23)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.38	0.03	0.38
(4,23)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.38	0.03	0.38
(1,174)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	10	0.37	0.05	0.38
(1,174)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	10	0.37	0.05	0.38
(2,493)	1:8:A:TYR:HA	1:11:A:TRP:HB2	10	0.37	0.05	0.38
(3,463)	1:8:A:TYR:HA	1:11:A:TRP:HB2	10	0.37	0.05	0.38
(1,409)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.37	0.0	0.37
(1,435)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	10	0.37	0.03	0.36
(1,501)	1:12:A:LEU:HA	1:16:A:GLY:HA2	10	0.37	0.07	0.37
(2,600)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	0.37	0.02	0.37
(2,600)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	0.37	0.02	0.37
(2,600)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	0.37	0.02	0.37
(4,35)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	0.37	0.02	0.37
(4,35)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	0.37	0.02	0.37
(4,35)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	0.37	0.02	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	10	0.37	0.0	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.37	0.0	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,471)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	10	0.36	0.05	0.38
(1,369)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.36	0.0	0.36
(2,139)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	10	0.36	0.07	0.35
(2,139)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	10	0.36	0.07	0.35
(3,130)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	10	0.36	0.07	0.35
(3,130)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	10	0.36	0.07	0.35
(1,377)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	10	0.36	0.0	0.36
(1,535)	1:9:A:ILE:HA	1:13:A:LYS:H	10	0.36	0.07	0.35
(1,332)	1:12:A:LEU:HB2	1:12:A:LEU:HG	10	0.36	0.01	0.36
(2,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.36	0.0	0.36
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	10	0.36	0.06	0.37
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	10	0.36	0.06	0.37
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	10	0.36	0.06	0.37
(3,110)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.36	0.0	0.36
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	10	0.36	0.06	0.37
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	10	0.36	0.06	0.37
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	10	0.36	0.06	0.37
(1,439)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.35	0.0	0.35
(1,291)	1:7:A:LEU:HD11	1:7:A:LEU:HG	10	0.35	0.0	0.35
(1,291)	1:7:A:LEU:HD12	1:7:A:LEU:HG	10	0.35	0.0	0.35
(1,291)	1:7:A:LEU:HD13	1:7:A:LEU:HG	10	0.35	0.0	0.35
(1,291)	1:7:A:LEU:HD21	1:7:A:LEU:HG	10	0.35	0.0	0.35
(1,291)	1:7:A:LEU:HD22	1:7:A:LEU:HG	10	0.35	0.0	0.35
(1,291)	1:7:A:LEU:HD23	1:7:A:LEU:HG	10	0.35	0.0	0.35
(1,228)	1:12:A:LEU:H	1:12:A:LEU:HB2	10	0.34	0.02	0.34
(2,15)	1:6:A:ARG:H	1:6:A:ARG:HG2	10	0.33	0.16	0.27
(4,2)	1:6:A:ARG:H	1:6:A:ARG:HG2	10	0.33	0.16	0.27
(1,420)	1:23:A:PRO:HA	1:23:A:PRO:HD3	10	0.33	0.05	0.35
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.33	0.0	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.33	0.0	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.33	0.0	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.33	0.0	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.33	0.0	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.33	0.0	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.32	0.06	0.32
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.32	0.06	0.32
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.32	0.06	0.32
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.32	0.06	0.32
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.32	0.06	0.32
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.32	0.06	0.32
(1,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.32	0.01	0.31
(1,97)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.31	0.02	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,114)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.31	0.02	0.3
(4,9)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.31	0.02	0.3
(1,324)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.31	0.0	0.31
(1,315)	1:10:A:GLN:HA	1:10:A:GLN:HB2	10	0.3	0.07	0.29
(1,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.3	0.09	0.3
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.3	0.03	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	10	0.3	0.03	0.28
(1,280)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	10	0.3	0.05	0.28
(1,247)	1:2:A:GLU:HA	1:2:A:GLU:HB3	10	0.3	0.07	0.3
(1,537)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	0.3	0.03	0.29
(1,537)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	0.3	0.03	0.29
(1,537)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	0.3	0.03	0.29
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	10	0.29	0.02	0.29
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	10	0.29	0.02	0.29
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	10	0.29	0.02	0.29
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	10	0.29	0.02	0.29
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	10	0.29	0.02	0.29
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	10	0.29	0.02	0.29
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	10	0.29	0.02	0.29
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	10	0.29	0.02	0.29
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	10	0.29	0.02	0.29
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	10	0.29	0.02	0.29
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	10	0.29	0.02	0.29
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	10	0.29	0.02	0.29
(1,304)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	10	0.29	0.0	0.29
(1,331)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.28	0.0	0.28
(1,512)	1:23:A:PRO:HA	1:24:A:PRO:HD2	10	0.28	0.03	0.29
(1,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.28	0.07	0.28
(1,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.28	0.07	0.28
(1,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.28	0.07	0.28
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	10	0.28	0.01	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	10	0.28	0.01	0.27
(1,495)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.27	0.06	0.25
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	10	0.27	0.01	0.26
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	10	0.27	0.01	0.26
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	10	0.27	0.01	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	10	0.27	0.01	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	10	0.27	0.01	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	10	0.27	0.01	0.26
(1,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	10	0.26	0.08	0.24
(1,355)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.26	0.0	0.26
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	10	0.26	0.03	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	10	0.26	0.03	0.27
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	10	0.26	0.03	0.27
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	10	0.26	0.03	0.27
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	10	0.26	0.03	0.27
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	10	0.26	0.03	0.27
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	10	0.26	0.03	0.27
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	10	0.26	0.03	0.27
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	10	0.26	0.03	0.27
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	10	0.26	0.03	0.27
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	10	0.26	0.03	0.27
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	10	0.26	0.03	0.27
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	10	0.26	0.03	0.27
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	10	0.26	0.03	0.27
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	10	0.26	0.03	0.27
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	10	0.26	0.03	0.27
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	10	0.26	0.03	0.27
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	10	0.26	0.03	0.27
(1,243)	1:11:A:TRP:HB3	1:12:A:LEU:H	10	0.26	0.03	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	10	0.26	0.0	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	10	0.26	0.0	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	10	0.26	0.0	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	10	0.26	0.0	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	10	0.26	0.0	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	10	0.26	0.0	0.26
(1,333)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.25	0.0	0.25
(1,333)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.25	0.0	0.25
(1,333)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.25	0.0	0.25
(2,107)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.25	0.02	0.26
(4,8)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.25	0.02	0.26
(1,469)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	10	0.25	0.01	0.25
(1,469)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	10	0.25	0.01	0.25
(1,469)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	10	0.25	0.01	0.25
(1,306)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	10	0.25	0.0	0.25
(1,306)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	10	0.25	0.0	0.25
(1,306)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	10	0.25	0.0	0.25
(2,185)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	10	0.25	0.02	0.25
(4,20)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	10	0.25	0.02	0.25
(1,285)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.24	0.0	0.24
(1,376)	1:19:A:SER:HB2	1:19:A:SER:HB3	10	0.24	0.0	0.24
(2,22)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.24	0.07	0.26
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.24	0.07	0.26
(1,325)	1:12:A:LEU:HA	1:12:A:LEU:HB3	10	0.24	0.01	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,292)	1:7:A:LEU:HB2	1:7:A:LEU:HG	10	0.24	0.04	0.24
(1,380)	1:21:A:ARG:HA	1:21:A:ARG:HB2	10	0.24	0.1	0.28
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD21	10	0.23	0.03	0.22
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD22	10	0.23	0.03	0.22
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD23	10	0.23	0.03	0.22
(1,55)	1:15:A:GLY:H	1:15:A:GLY:HA2	10	0.22	0.03	0.24
(1,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.21	0.01	0.21
(1,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	10	0.2	0.03	0.2
(1,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	10	0.2	0.03	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.2	0.0	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.2	0.0	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.2	0.0	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.2	0.0	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.2	0.0	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.2	0.0	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.2	0.0	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.2	0.0	0.2
(1,511)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.2	0.04	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	10	0.2	0.01	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	10	0.2	0.01	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	10	0.2	0.01	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	10	0.2	0.01	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	10	0.2	0.01	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	10	0.2	0.01	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	10	0.2	0.01	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	10	0.2	0.01	0.2
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.19	0.02	0.2
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.19	0.02	0.2
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.19	0.02	0.2
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.19	0.02	0.2
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.19	0.02	0.2
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.19	0.02	0.2
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.19	0.02	0.2
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.19	0.02	0.2
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.19	0.02	0.2
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.19	0.02	0.2
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.19	0.02	0.2
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.19	0.02	0.2
(1,361)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.19	0.0	0.19
(1,254)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	10	0.19	0.0	0.19
(1,353)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	10	0.19	0.0	0.19
(1,452)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	10	0.19	0.0	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,460)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	10	0.19	0.0	0.19
(2,184)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	0.19	0.02	0.18
(2,184)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	0.19	0.02	0.18
(4,19)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	0.19	0.02	0.18
(4,19)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	0.19	0.02	0.18
(1,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.18	0.03	0.2
(1,260)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	10	0.18	0.0	0.18
(1,441)	1:24:A:PRO:HA	1:24:A:PRO:HB3	10	0.18	0.01	0.17
(1,293)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.17	0.0	0.17
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	10	0.17	0.03	0.18
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	10	0.17	0.03	0.18
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	10	0.17	0.03	0.18
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	10	0.17	0.03	0.18
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	10	0.17	0.03	0.18
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	10	0.17	0.03	0.18
(1,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.17	0.01	0.17
(1,298)	1:9:A:ILE:HA	1:9:A:ILE:HG13	10	0.17	0.02	0.17
(1,86)	1:14:A:ASP:H	1:15:A:GLY:H	10	0.16	0.02	0.16
(1,399)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	10	0.16	0.0	0.16
(1,374)	1:19:A:SER:HA	1:19:A:SER:HB2	10	0.16	0.03	0.17
(1,426)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.15	0.03	0.14
(1,140)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	10	0.15	0.01	0.15
(1,51)	1:20:A:GLY:H	1:20:A:GLY:HA2	10	0.15	0.01	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	10	0.14	0.01	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	10	0.14	0.01	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	10	0.14	0.01	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	10	0.14	0.01	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	10	0.14	0.01	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	10	0.14	0.01	0.14
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	10	0.14	0.01	0.14
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	10	0.14	0.01	0.14
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	10	0.14	0.01	0.14
(1,390)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	10	0.14	0.01	0.15
(1,445)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	10	0.14	0.01	0.14
(1,50)	1:9:A:ILE:H	1:9:A:ILE:HB	10	0.13	0.01	0.13
(1,509)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	10	0.12	0.0	0.12
(1,334)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.12	0.0	0.12
(1,334)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.12	0.0	0.12
(1,334)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.12	0.0	0.12
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB2	10	0.1	0.0	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB3	10	0.1	0.0	0.1
(1,313)	1:10:A:GLN:HA	1:10:A:GLN:HG3	9	0.55	0.09	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,540)	1:2:A:GLU:HB2	1:6:A:ARG:H	9	0.54	0.2	0.55
(1,123)	1:23:A:PRO:HB2	1:25:A:CYS:H	9	0.46	0.14	0.43
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	9	0.44	0.07	0.45
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	9	0.44	0.07	0.45
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	9	0.44	0.07	0.45
(1,90)	1:10:A:GLN:HB3	1:11:A:TRP:H	9	0.41	0.15	0.4
(2,177)	1:23:A:PRO:HB3	1:25:A:CYS:H	9	0.39	0.18	0.37
(3,160)	1:23:A:PRO:HB3	1:25:A:CYS:H	9	0.39	0.18	0.37
(1,523)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	9	0.34	0.03	0.35
(1,207)	1:8:A:TYR:HD1	1:25:A:CYS:H	9	0.34	0.09	0.33
(1,207)	1:8:A:TYR:HD2	1:25:A:CYS:H	9	0.34	0.09	0.33
(2,457)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	9	0.31	0.09	0.28
(3,427)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	9	0.31	0.09	0.28
(2,515)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.29	0.05	0.29
(3,485)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.29	0.05	0.29
(1,214)	1:15:A:GLY:H	1:16:A:GLY:H	9	0.25	0.06	0.23
(1,518)	1:1:A:GLU:HA	1:1:A:GLU:HB2	9	0.21	0.19	0.11
(1,92)	1:7:A:LEU:H	1:7:A:LEU:HG	9	0.2	0.04	0.18
(1,356)	1:17:A:PRO:HA	1:17:A:PRO:HD2	9	0.17	0.03	0.18
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	9	0.17	0.03	0.17
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	9	0.17	0.03	0.17
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	9	0.17	0.03	0.17
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	9	0.17	0.03	0.17
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	9	0.17	0.03	0.17
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	9	0.17	0.03	0.17
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	9	0.17	0.03	0.17
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	9	0.17	0.03	0.17
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	9	0.17	0.03	0.17
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	9	0.17	0.03	0.17
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	9	0.17	0.03	0.17
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	9	0.17	0.03	0.17
(1,489)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	9	0.17	0.05	0.15
(1,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	9	0.14	0.03	0.15
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	8	1.28	0.13	1.28
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	8	1.28	0.13	1.28
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	8	1.28	0.13	1.28
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	8	1.28	0.13	1.28
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	8	1.28	0.13	1.28
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	8	1.28	0.13	1.28
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	8	0.93	0.32	0.77
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	8	0.93	0.32	0.77
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	8	0.93	0.32	0.77

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	8	0.88	0.06	0.88
(3,161)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	8	0.88	0.06	0.88
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	8	0.82	0.1	0.83
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	8	0.82	0.1	0.83
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	8	0.82	0.1	0.83
(2,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	8	0.78	0.2	0.7
(3,162)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	8	0.78	0.2	0.7
(1,270)	1:6:A:ARG:HA	1:6:A:ARG:HG2	8	0.71	0.14	0.78
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	8	0.68	0.13	0.68
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	8	0.68	0.13	0.68
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	8	0.68	0.13	0.68
(2,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	8	0.64	0.27	0.48
(3,548)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	8	0.64	0.27	0.48
(1,483)	1:7:A:LEU:HA	1:10:A:GLN:HB3	8	0.56	0.05	0.56
(1,571)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	8	0.47	0.28	0.39
(1,571)	1:24:A:PRO:HG3	1:25:A:CYS:HB2	8	0.47	0.28	0.39
(2,89)	1:10:A:GLN:HB2	1:11:A:TRP:H	8	0.44	0.02	0.44
(3,84)	1:10:A:GLN:HB2	1:11:A:TRP:H	8	0.44	0.02	0.44
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	8	0.42	0.19	0.41
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	8	0.42	0.19	0.41
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	8	0.42	0.19	0.41
(1,274)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	8	0.4	0.26	0.26
(1,430)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	8	0.4	0.06	0.4
(1,385)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	8	0.36	0.13	0.42
(1,38)	1:21:A:ARG:H	1:21:A:ARG:HB2	8	0.34	0.09	0.34
(2,367)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	8	0.34	0.0	0.34
(3,339)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	8	0.34	0.0	0.34
(1,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	8	0.34	0.07	0.34
(1,539)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	8	0.32	0.07	0.32
(2,222)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	8	0.26	0.03	0.26
(3,202)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	8	0.26	0.03	0.26
(2,197)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.25	0.06	0.24
(3,177)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.25	0.06	0.24
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG2	8	0.24	0.03	0.24
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG3	8	0.24	0.03	0.24
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	8	0.23	0.06	0.24
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	8	0.23	0.06	0.24
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	8	0.23	0.06	0.24
(1,252)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	8	0.23	0.03	0.22
(1,125)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	8	0.2	0.08	0.16
(1,95)	1:6:A:ARG:HB2	1:7:A:LEU:H	8	0.2	0.03	0.19
(1,95)	1:6:A:ARG:HB3	1:7:A:LEU:H	8	0.2	0.03	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,488)	1:8:A:TYR:HA	1:11:A:TRP:HB3	8	0.19	0.04	0.19
(1,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	8	0.19	0.05	0.21
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD11	8	0.12	0.01	0.12
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD12	8	0.12	0.01	0.12
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD13	8	0.12	0.01	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD11	8	0.12	0.01	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD12	8	0.12	0.01	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD13	8	0.12	0.01	0.12
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	7	0.95	0.03	0.94
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	7	0.95	0.03	0.94
(1,273)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	7	0.64	0.16	0.69
(1,267)	1:6:A:ARG:HA	1:6:A:ARG:HD3	7	0.62	0.21	0.68
(1,554)	1:4:A:CYS:HA	1:7:A:LEU:HG	7	0.45	0.21	0.55
(1,60)	1:25:A:CYS:H	1:25:A:CYS:HB2	7	0.4	0.11	0.47
(2,375)	1:19:A:SER:HA	1:19:A:SER:HB3	7	0.35	0.0	0.35
(3,347)	1:19:A:SER:HA	1:19:A:SER:HB3	7	0.35	0.0	0.35
(1,312)	1:10:A:GLN:HA	1:10:A:GLN:HG2	7	0.26	0.15	0.18
(1,384)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	7	0.26	0.11	0.26
(1,568)	1:19:A:SER:HB3	1:21:A:ARG:HB3	7	0.24	0.11	0.27
(1,259)	1:4:A:CYS:HA	1:4:A:CYS:HB2	7	0.23	0.09	0.21
(2,198)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	7	0.22	0.05	0.21
(3,178)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	7	0.22	0.05	0.21
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	7	0.19	0.05	0.19
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	7	0.19	0.05	0.19
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	7	0.19	0.05	0.19
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	7	0.19	0.05	0.19
(1,458)	1:25:A:CYS:HA	1:25:A:CYS:HB3	7	0.17	0.03	0.15
(2,16)	1:6:A:ARG:H	1:6:A:ARG:HG3	7	0.17	0.05	0.15
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG3	7	0.17	0.05	0.15
(1,553)	1:22:A:PRO:HA	1:23:A:PRO:HG2	7	0.14	0.01	0.14
(1,581)	1:1:A:GLU:HB3	1:2:A:GLU:HG2	6	0.6	0.2	0.64
(1,558)	1:2:A:GLU:HA	1:5:A:VAL:HB	6	0.58	0.51	0.29
(1,522)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	6	0.47	0.02	0.47
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG2	6	0.34	0.14	0.42
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	6	0.34	0.14	0.42
(1,481)	1:7:A:LEU:HA	1:10:A:GLN:HB2	6	0.32	0.09	0.31
(1,248)	1:2:A:GLU:HA	1:2:A:GLU:HG2	6	0.3	0.16	0.24
(1,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	6	0.29	0.19	0.18
(1,387)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	6	0.23	0.06	0.2
(1,121)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.2	0.04	0.18
(2,455)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	6	0.2	0.1	0.18
(3,425)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	6	0.2	0.1	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	6	0.13	0.02	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	6	0.13	0.02	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	6	0.13	0.02	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	6	0.13	0.02	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	6	0.13	0.02	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	6	0.13	0.02	0.14
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG11	6	0.11	0.01	0.11
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG12	6	0.11	0.01	0.11
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG13	6	0.11	0.01	0.11
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG11	6	0.11	0.01	0.11
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG12	6	0.11	0.01	0.11
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG13	6	0.11	0.01	0.11
(1,54)	1:18:A:SER:H	1:18:A:SER:HB3	5	0.67	0.05	0.69
(1,372)	1:18:A:SER:HA	1:18:A:SER:HB2	5	0.46	0.02	0.47
(1,371)	1:18:A:SER:HA	1:18:A:SER:HB3	5	0.38	0.02	0.37
(1,525)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	5	0.35	0.03	0.35
(2,186)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	5	0.23	0.03	0.22
(2,186)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	5	0.23	0.03	0.22
(3,166)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	5	0.23	0.03	0.22
(3,166)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	5	0.23	0.03	0.22
(1,465)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	5	0.2	0.03	0.21
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	5	0.19	0.07	0.17
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	5	0.19	0.07	0.17
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.19	0.01	0.19
(3,26)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.19	0.01	0.19
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	5	0.18	0.07	0.16
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	5	0.18	0.07	0.16
(1,408)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	5	0.11	0.0	0.11
(2,281)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	5	0.11	0.01	0.11
(3,257)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	5	0.11	0.01	0.11
(2,482)	1:3:A:GLU:HA	1:6:A:ARG:HB3	4	0.74	0.22	0.63
(3,452)	1:3:A:GLU:HA	1:6:A:ARG:HB3	4	0.74	0.22	0.63
(1,276)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	4	0.66	0.25	0.71
(1,36)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	4	0.49	0.01	0.5
(1,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	4	0.43	0.1	0.41
(2,477)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	4	0.42	0.03	0.42
(3,447)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	4	0.42	0.03	0.42
(1,541)	1:2:A:GLU:HB3	1:6:A:ARG:H	4	0.34	0.11	0.32
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD11	4	0.26	0.08	0.24
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD12	4	0.26	0.08	0.24
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD13	4	0.26	0.08	0.24
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD21	4	0.26	0.08	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD22	4	0.26	0.08	0.24
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD23	4	0.26	0.08	0.24
(2,98)	1:7:A:LEU:H	1:10:A:GLN:HB2	4	0.23	0.09	0.19
(3,91)	1:7:A:LEU:H	1:10:A:GLN:HB2	4	0.23	0.09	0.19
(1,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	4	0.22	0.1	0.22
(1,506)	1:18:A:SER:HB2	1:19:A:SER:H	4	0.21	0.08	0.2
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	4	0.2	0.06	0.16
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	4	0.2	0.06	0.16
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	4	0.2	0.06	0.16
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	4	0.2	0.06	0.16
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	4	0.2	0.06	0.16
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	4	0.2	0.06	0.16
(2,225)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	4	0.14	0.02	0.15
(3,205)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	4	0.14	0.02	0.15
(1,548)	1:12:A:LEU:H	1:14:A:ASP:H	4	0.14	0.03	0.13
(1,64)	1:19:A:SER:H	1:19:A:SER:HB2	4	0.13	0.02	0.14
(1,65)	1:19:A:SER:H	1:19:A:SER:HB3	4	0.12	0.02	0.12
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	4	0.12	0.01	0.12
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	4	0.12	0.01	0.12
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	4	0.12	0.01	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD11	4	0.12	0.0	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD12	4	0.12	0.0	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD13	4	0.12	0.0	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD11	4	0.12	0.0	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD12	4	0.12	0.0	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD13	4	0.12	0.0	0.12
(1,221)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	3	1.58	0.03	1.57
(2,566)	1:6:A:ARG:HD2	1:7:A:LEU:HG	3	1.36	0.16	1.47
(3,534)	1:6:A:ARG:HD2	1:7:A:LEU:HG	3	1.36	0.16	1.47
(1,566)	1:6:A:ARG:HD2	1:7:A:LEU:HG	3	0.82	0.16	0.93
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG11	3	0.81	0.5	0.88
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG12	3	0.81	0.5	0.88
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG13	3	0.81	0.5	0.88
(1,580)	1:11:A:TRP:HB2	1:21:A:ARG:HD2	3	0.6	0.11	0.64
(1,508)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	3	0.51	0.18	0.59
(1,508)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	3	0.51	0.18	0.59
(1,508)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	3	0.51	0.18	0.59
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD11	3	0.46	0.23	0.3
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD12	3	0.46	0.23	0.3
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD13	3	0.46	0.23	0.3
(1,576)	1:10:A:GLN:HG2	1:11:A:TRP:HA	3	0.43	0.1	0.41
(1,271)	1:6:A:ARG:HA	1:6:A:ARG:HG3	3	0.43	0.06	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,217)	1:10:A:GLN:HG2	1:11:A:TRP:H	3	0.41	0.08	0.35
(1,386)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	3	0.37	0.02	0.37
(2,508)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	3	0.32	0.1	0.28
(2,508)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	3	0.32	0.1	0.28
(2,508)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	3	0.32	0.1	0.28
(3,478)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	3	0.32	0.1	0.28
(3,478)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	3	0.32	0.1	0.28
(3,478)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	3	0.32	0.1	0.28
(1,245)	1:11:A:TRP:H	1:12:A:LEU:H	3	0.2	0.03	0.22
(2,41)	1:21:A:ARG:H	1:21:A:ARG:HD3	3	0.2	0.01	0.19
(3,37)	1:21:A:ARG:H	1:21:A:ARG:HD3	3	0.2	0.01	0.19
(1,157)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	3	0.18	0.08	0.15
(1,157)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	3	0.18	0.08	0.15
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG21	3	0.18	0.05	0.19
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG22	3	0.18	0.05	0.19
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG23	3	0.18	0.05	0.19
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG21	3	0.18	0.05	0.19
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG22	3	0.18	0.05	0.19
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG23	3	0.18	0.05	0.19
(2,282)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	3	0.18	0.01	0.18
(4,25)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	3	0.18	0.01	0.18
(2,387)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	3	0.18	0.02	0.18
(3,359)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	3	0.18	0.02	0.18
(2,23)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.14	0.02	0.13
(4,3)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.14	0.02	0.13
(1,359)	1:17:A:PRO:HA	1:17:A:PRO:HG2	3	0.12	0.01	0.12
(1,359)	1:17:A:PRO:HA	1:17:A:PRO:HG3	3	0.12	0.01	0.12
(1,37)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	3	0.11	0.01	0.11
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	3	0.11	0.0	0.11
(1,590)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	2	0.8	0.24	0.8
(1,590)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	2	0.8	0.24	0.8
(1,590)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	2	0.8	0.24	0.8
(2,37)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	2	0.56	0.0	0.56
(3,33)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	2	0.56	0.0	0.56
(1,67)	1:3:A:GLU:H	1:3:A:GLU:HA	2	0.54	0.0	0.54
(1,559)	1:19:A:SER:HB2	1:21:A:ARG:HB2	2	0.52	0.35	0.52
(1,556)	1:2:A:GLU:HA	1:5:A:VAL:HG11	2	0.49	0.23	0.49
(1,556)	1:2:A:GLU:HA	1:5:A:VAL:HG12	2	0.49	0.23	0.49
(1,556)	1:2:A:GLU:HA	1:5:A:VAL:HG13	2	0.49	0.23	0.49
(1,555)	1:2:A:GLU:HA	1:5:A:VAL:HG21	2	0.46	0.29	0.46
(1,555)	1:2:A:GLU:HA	1:5:A:VAL:HG22	2	0.46	0.29	0.46
(1,555)	1:2:A:GLU:HA	1:5:A:VAL:HG23	2	0.46	0.29	0.46

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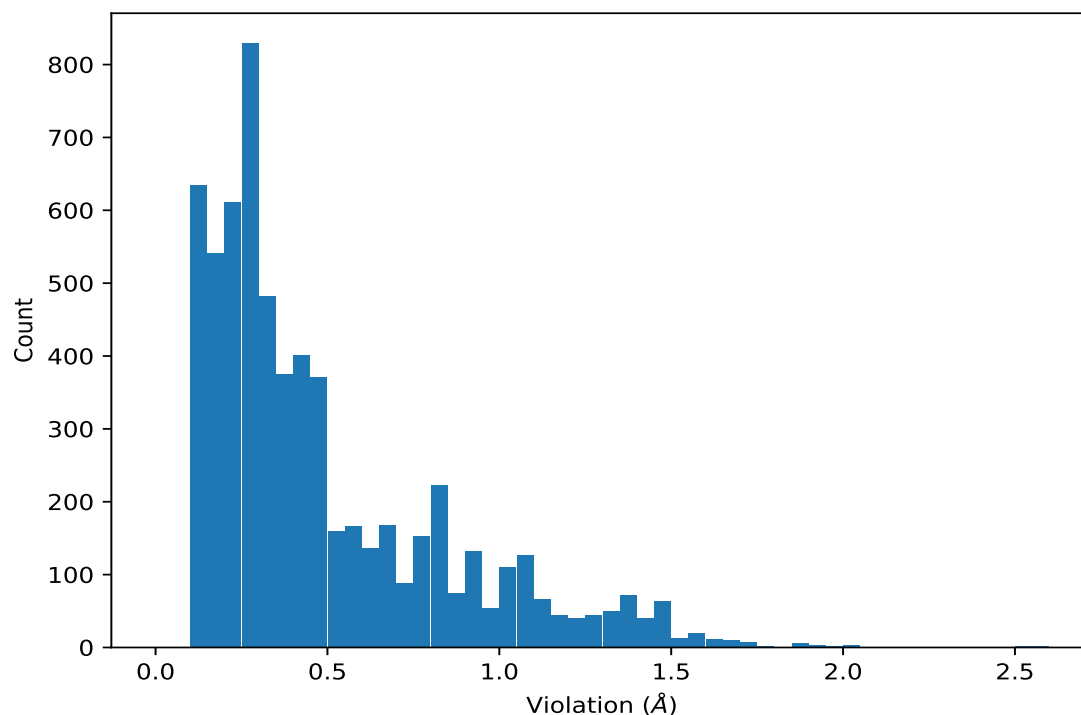
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,547)	1:11:A:TRP:HH2	1:17:A:PRO:HB3	2	0.46	0.01	0.46
(2,118)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	2	0.44	0.03	0.44
(3,109)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	2	0.44	0.03	0.44
(1,482)	1:3:A:GLU:HA	1:6:A:ARG:HB3	2	0.38	0.16	0.38
(1,570)	1:24:A:PRO:HB2	1:25:A:CYS:HB2	2	0.38	0.26	0.38
(1,269)	1:6:A:ARG:HA	1:6:A:ARG:HB2	2	0.36	0.04	0.36
(1,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	2	0.33	0.02	0.33
(1,528)	1:16:A:GLY:H	1:19:A:SER:HB3	2	0.32	0.1	0.32
(2,195)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	2	0.32	0.01	0.32
(3,175)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	2	0.32	0.01	0.32
(2,35)	1:4:A:CYS:HB2	1:5:A:VAL:H	2	0.31	0.05	0.31
(3,31)	1:4:A:CYS:HB2	1:5:A:VAL:H	2	0.31	0.05	0.31
(1,61)	1:25:A:CYS:H	1:25:A:CYS:HB3	2	0.22	0.12	0.22
(2,156)	1:11:A:TRP:HZ3	1:23:A:PRO:HB2	2	0.22	0.02	0.22
(3,143)	1:11:A:TRP:HZ3	1:23:A:PRO:HB2	2	0.22	0.02	0.22
(1,567)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	2	0.18	0.02	0.18
(1,401)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	2	0.17	0.04	0.17
(2,416)	1:23:A:PRO:HA	1:23:A:PRO:HG3	2	0.16	0.01	0.16
(3,388)	1:23:A:PRO:HA	1:23:A:PRO:HG3	2	0.16	0.01	0.16
(1,108)	1:19:A:SER:HB2	1:21:A:ARG:H	2	0.15	0.0	0.15
(2,201)	1:15:A:GLY:HA3	1:16:A:GLY:H	2	0.14	0.03	0.14
(3,181)	1:15:A:GLY:HA3	1:16:A:GLY:H	2	0.14	0.03	0.14
(1,42)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.14	0.02	0.14
(2,221)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	2	0.14	0.02	0.14
(3,201)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	2	0.14	0.02	0.14
(1,251)	1:2:A:GLU:HB3	1:2:A:GLU:HG2	2	0.12	0.01	0.12
(1,368)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	2	0.12	0.01	0.12
(1,368)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	2	0.12	0.01	0.12
(1,128)	1:8:A:TYR:HA	1:8:A:TYR:HD1	2	0.11	0.0	0.11
(1,128)	1:8:A:TYR:HA	1:8:A:TYR:HD2	2	0.11	0.0	0.11
(1,130)	1:5:A:VAL:HA	1:8:A:TYR:HD1	2	0.11	0.01	0.11
(1,130)	1:5:A:VAL:HA	1:8:A:TYR:HD2	2	0.11	0.01	0.11
(1,329)	1:12:A:LEU:HA	1:12:A:LEU:HD11	2	0.11	0.0	0.11
(1,329)	1:12:A:LEU:HA	1:12:A:LEU:HD12	2	0.11	0.0	0.11
(1,329)	1:12:A:LEU:HA	1:12:A:LEU:HD13	2	0.11	0.0	0.11
(1,392)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	2	0.11	0.0	0.11
(1,392)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,29)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	7	2.57
(2,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	7	2.57
(4,29)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	6	2.55
(2,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	6	2.55
(1,520)	1:1:A:GLU:HA	1:1:A:GLU:HG2	10	2.35
(1,520)	1:1:A:GLU:HA	1:1:A:GLU:HG2	8	2.29
(1,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	7	2.04
(4,5)	1:9:A:ILE:HB	1:11:A:TRP:H	5	2.03
(2,88)	1:9:A:ILE:HB	1:11:A:TRP:H	5	2.03
(1,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	6	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,5)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.97
(2,88)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.97
(1,520)	1:1:A:GLU:HA	1:1:A:GLU:HG2	5	1.93
(4,5)	1:9:A:ILE:HB	1:11:A:TRP:H	8	1.91
(2,88)	1:9:A:ILE:HB	1:11:A:TRP:H	8	1.91
(1,520)	1:1:A:GLU:HA	1:1:A:GLU:HG2	2	1.91
(4,5)	1:9:A:ILE:HB	1:11:A:TRP:H	2	1.89
(2,88)	1:9:A:ILE:HB	1:11:A:TRP:H	2	1.89
(4,5)	1:9:A:ILE:HB	1:11:A:TRP:H	3	1.86
(2,88)	1:9:A:ILE:HB	1:11:A:TRP:H	3	1.86
(4,5)	1:9:A:ILE:HB	1:11:A:TRP:H	6	1.85
(2,88)	1:9:A:ILE:HB	1:11:A:TRP:H	6	1.85
(1,520)	1:1:A:GLU:HA	1:1:A:GLU:HG2	1	1.81
(4,5)	1:9:A:ILE:HB	1:11:A:TRP:H	1	1.79
(2,88)	1:9:A:ILE:HB	1:11:A:TRP:H	1	1.79
(4,29)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	1	1.74
(2,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	1	1.74
(4,5)	1:9:A:ILE:HB	1:11:A:TRP:H	9	1.73
(2,88)	1:9:A:ILE:HB	1:11:A:TRP:H	9	1.73
(1,520)	1:1:A:GLU:HA	1:1:A:GLU:HG2	3	1.72
(1,520)	1:1:A:GLU:HA	1:1:A:GLU:HG2	6	1.72
(1,521)	1:1:A:GLU:HA	1:1:A:GLU:HG3	3	1.71
(1,521)	1:1:A:GLU:HA	1:1:A:GLU:HG3	5	1.68
(1,521)	1:1:A:GLU:HA	1:1:A:GLU:HG3	9	1.68
(4,5)	1:9:A:ILE:HB	1:11:A:TRP:H	4	1.67
(2,88)	1:9:A:ILE:HB	1:11:A:TRP:H	4	1.67
(4,5)	1:9:A:ILE:HB	1:11:A:TRP:H	7	1.66
(2,88)	1:9:A:ILE:HB	1:11:A:TRP:H	7	1.66
(1,563)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	1	1.66
(1,563)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	1	1.66
(1,563)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	3	1.66
(1,563)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	3	1.66
(1,563)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	6	1.65
(1,563)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	6	1.65
(1,563)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	8	1.64
(1,563)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	8	1.64
(1,563)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	9	1.64
(1,563)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	9	1.64
(4,29)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	1.63
(2,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	1.63
(1,221)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	5	1.62
(3,454)	1:4:A:CYS:HA	1:7:A:LEU:HB3	7	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	7	1.61
(1,520)	1:1:A:GLU:HA	1:1:A:GLU:HG2	7	1.61
(1,563)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	4	1.59
(1,563)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	4	1.59
(1,563)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	10	1.59
(1,563)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	10	1.59
(4,29)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	2	1.58
(2,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	2	1.58
(1,563)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	2	1.58
(1,563)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	2	1.58
(4,29)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	8	1.57
(4,29)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	9	1.57
(2,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	8	1.57
(2,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	9	1.57
(1,563)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	5	1.57
(1,563)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	5	1.57
(1,563)	1:8:A:TYR:HB2	1:9:A:ILE:HG13	7	1.57
(1,563)	1:8:A:TYR:HB3	1:9:A:ILE:HG13	7	1.57
(1,549)	1:20:A:GLY:H	1:21:A:ARG:H	3	1.57
(1,549)	1:20:A:GLY:H	1:21:A:ARG:H	8	1.57
(1,221)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	2	1.57
(1,221)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	3	1.55
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	10	1.53
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	10	1.53
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	10	1.53
(1,549)	1:20:A:GLY:H	1:21:A:ARG:H	7	1.53
(4,29)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	4	1.51
(2,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	4	1.51
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	5	1.5
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	5	1.5
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	5	1.5
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	5	1.5
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	5	1.5
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	5	1.5
(1,558)	1:2:A:GLU:HA	1:5:A:VAL:HB	6	1.5
(4,29)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	3	1.49
(4,29)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	5	1.49
(2,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	3	1.49
(2,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	5	1.49
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	5	1.49
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	5	1.49
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	5	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,534)	1:6:A:ARG:HD2	1:7:A:LEU:HG	10	1.48
(2,566)	1:6:A:ARG:HD2	1:7:A:LEU:HG	10	1.48
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	8	1.48
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	8	1.48
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	8	1.48
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	9	1.48
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	9	1.48
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	9	1.48
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	10	1.48
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	10	1.48
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	10	1.48
(3,534)	1:6:A:ARG:HD2	1:7:A:LEU:HG	1	1.47
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	4	1.47
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	4	1.47
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	4	1.47
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	5	1.47
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	5	1.47
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	5	1.47
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	7	1.47
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	7	1.47
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	7	1.47
(2,566)	1:6:A:ARG:HD2	1:7:A:LEU:HG	1	1.47
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	4	1.47
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	4	1.47
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	4	1.47
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	5	1.47
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	5	1.47
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	5	1.47
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	7	1.47
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	7	1.47
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	7	1.47
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	4	1.47
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	4	1.47
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	4	1.47
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	2	1.46
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	2	1.46
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	2	1.46
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	10	1.46
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	10	1.46
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	10	1.46
(3,454)	1:4:A:CYS:HA	1:7:A:LEU:HB3	4	1.46
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	2	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	2	1.46
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	2	1.46
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	10	1.46
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	10	1.46
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	10	1.46
(2,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	4	1.46
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	1	1.46
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	1	1.46
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	1	1.46
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	2	1.46
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	2	1.46
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	2	1.46
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	3	1.46
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	3	1.46
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	3	1.46
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	1	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	1	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	1	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	3	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	3	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	3	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	6	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	6	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	6	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	8	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	8	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	8	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	9	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	9	1.45
(3,486)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	9	1.45
(3,454)	1:4:A:CYS:HA	1:7:A:LEU:HB3	8	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	1	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	1	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	1	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	3	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	3	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	3	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	6	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	6	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	6	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	8	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	8	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	8	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG21	9	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG22	9	1.45
(2,516)	1:8:A:TYR:HB2	1:9:A:ILE:HG23	9	1.45
(2,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	8	1.45
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	6	1.45
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	6	1.45
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	6	1.45
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	7	1.45
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	7	1.45
(1,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	7	1.45
(1,88)	1:9:A:ILE:HB	1:11:A:TRP:H	5	1.43
(1,520)	1:1:A:GLU:HA	1:1:A:GLU:HG2	4	1.41
(3,129)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	1.4
(3,129)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	1.4
(3,129)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	1.4
(3,129)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	1.4
(3,129)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	1.4
(3,129)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	1.4
(3,129)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	1.4
(2,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	1.4
(2,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	1.4
(2,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	1.4
(2,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	1.4
(2,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	1.4
(2,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	1.4
(2,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	1.4
(1,549)	1:20:A:GLY:H	1:21:A:ARG:H	6	1.4
(1,394)	1:22:A:PRO:HA	1:22:A:PRO:HD3	6	1.4
(3,129)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	1.39
(3,129)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.39
(2,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	1.39
(2,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.39
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	9	1.39
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	9	1.39
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	9	1.39
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	9	1.39
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	9	1.39
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	9	1.39
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	1	1.38
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	1	1.38
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	1	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,129)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	1.38
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	1	1.38
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	1	1.38
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	1	1.38
(2,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	1.38
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	8	1.38
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	8	1.38
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	8	1.38
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	8	1.38
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	8	1.38
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	8	1.38
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG11	6	1.38
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG12	6	1.38
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG13	6	1.38
(1,490)	1:14:A:ASP:HB3	1:19:A:SER:HB2	9	1.38
(3,124)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	3	1.37
(3,124)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	5	1.37
(2,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	3	1.37
(2,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	5	1.37
(1,549)	1:20:A:GLY:H	1:21:A:ARG:H	5	1.37
(3,454)	1:4:A:CYS:HA	1:7:A:LEU:HB3	10	1.36
(3,124)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	4	1.36
(2,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	10	1.36
(2,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	4	1.36
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	1	1.36
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	1	1.36
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	1	1.36
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	1	1.36
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	1	1.36
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	1	1.36
(1,88)	1:9:A:ILE:HB	1:11:A:TRP:H	10	1.36
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	2	1.35
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	2	1.35
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	2	1.35
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	4	1.35
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	4	1.35
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	4	1.35
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	2	1.35
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	2	1.35
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	2	1.35
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	4	1.35
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	4	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	4	1.35
(3,124)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	2	1.34
(3,124)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	6	1.34
(3,124)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	8	1.34
(2,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	2	1.34
(2,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	6	1.34
(2,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	8	1.34
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	7	1.34
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	7	1.34
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	7	1.34
(1,394)	1:22:A:PRO:HA	1:22:A:PRO:HD3	1	1.34
(3,454)	1:4:A:CYS:HA	1:7:A:LEU:HB3	5	1.33
(3,124)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	9	1.33
(2,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	5	1.33
(2,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	9	1.33
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	6	1.33
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	6	1.33
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	6	1.33
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	6	1.33
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	6	1.33
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	6	1.33
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	10	1.33
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	10	1.33
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	10	1.33
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	10	1.33
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	10	1.33
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	10	1.33
(1,549)	1:20:A:GLY:H	1:21:A:ARG:H	10	1.33
(1,394)	1:22:A:PRO:HA	1:22:A:PRO:HD3	2	1.33
(1,394)	1:22:A:PRO:HA	1:22:A:PRO:HD3	5	1.33
(1,394)	1:22:A:PRO:HA	1:22:A:PRO:HD3	7	1.33
(1,394)	1:22:A:PRO:HA	1:22:A:PRO:HD3	9	1.33
(3,140)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	4	1.32
(3,140)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	4	1.32
(2,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	4	1.32
(2,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	4	1.32
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	7	1.32
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	7	1.32
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	7	1.32
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	7	1.32
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	7	1.32
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	7	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:20:A:GLY:H	1:21:A:ARG:H	4	1.32
(3,124)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	7	1.31
(2,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	7	1.31
(1,490)	1:14:A:ASP:HB3	1:19:A:SER:HB2	8	1.31
(1,466)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	3	1.31
(1,549)	1:20:A:GLY:H	1:21:A:ARG:H	1	1.3
(1,466)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	5	1.3
(1,466)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	1.3
(1,88)	1:9:A:ILE:HB	1:11:A:TRP:H	8	1.3
(3,454)	1:4:A:CYS:HA	1:7:A:LEU:HB3	9	1.29
(2,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	9	1.29
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	5	1.29
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	5	1.29
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	5	1.29
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	5	1.29
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	5	1.29
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	5	1.29
(1,88)	1:9:A:ILE:HB	1:11:A:TRP:H	2	1.29
(3,140)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	7	1.28
(3,140)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	7	1.28
(3,140)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	8	1.28
(3,140)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	8	1.28
(2,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	7	1.28
(2,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	7	1.28
(2,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	8	1.28
(2,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	8	1.28
(1,466)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	4	1.28
(1,466)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	8	1.28
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	3	1.27
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	3	1.27
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	3	1.27
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	3	1.27
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	3	1.27
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	3	1.27
(1,466)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	1	1.27
(1,549)	1:20:A:GLY:H	1:21:A:ARG:H	2	1.26
(1,394)	1:22:A:PRO:HA	1:22:A:PRO:HD3	4	1.26
(1,394)	1:22:A:PRO:HA	1:22:A:PRO:HD3	8	1.26
(1,88)	1:9:A:ILE:HB	1:11:A:TRP:H	3	1.26
(3,140)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	2	1.25
(3,140)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	2	1.25
(3,140)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	6	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,140)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	6	1.25
(3,140)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	1.25
(3,140)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	1.25
(2,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	2	1.25
(2,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	2	1.25
(2,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	6	1.25
(2,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	6	1.25
(2,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	1.25
(2,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	1.25
(1,466)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	6	1.25
(1,466)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	7	1.25
(1,394)	1:22:A:PRO:HA	1:22:A:PRO:HD3	10	1.25
(3,140)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	1.24
(3,140)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	1.24
(2,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	1.24
(2,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	1.24
(1,490)	1:14:A:ASP:HB3	1:19:A:SER:HB2	5	1.24
(1,394)	1:22:A:PRO:HA	1:22:A:PRO:HD3	3	1.24
(1,88)	1:9:A:ILE:HB	1:11:A:TRP:H	6	1.24
(3,140)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	5	1.23
(3,140)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	5	1.23
(2,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	5	1.23
(2,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	5	1.23
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	4	1.23
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	4	1.23
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	4	1.23
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	4	1.23
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	4	1.23
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	4	1.23
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	8	1.22
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	8	1.22
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	8	1.22
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	9	1.22
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	9	1.22
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	9	1.22
(3,140)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	1	1.22
(3,140)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	1	1.22
(3,140)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	3	1.22
(3,140)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	3	1.22
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	8	1.22
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	8	1.22
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	8	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	9	1.22
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	9	1.22
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	9	1.22
(2,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	1	1.22
(2,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	1	1.22
(2,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	3	1.22
(2,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	3	1.22
(1,549)	1:20:A:GLY:H	1:21:A:ARG:H	9	1.22
(3,454)	1:4:A:CYS:HA	1:7:A:LEU:HB3	2	1.21
(2,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	2	1.21
(4,18)	1:11:A:TRP:HE3	1:12:A:LEU:HG	7	1.2
(3,454)	1:4:A:CYS:HA	1:7:A:LEU:HB3	3	1.2
(3,124)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	1.2
(2,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	3	1.2
(2,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	7	1.2
(2,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	1.2
(1,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	1	1.2
(4,18)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	1.19
(3,548)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	4	1.19
(2,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	4	1.19
(2,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	1.19
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	2	1.19
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	2	1.19
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	2	1.19
(1,610)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	2	1.19
(1,610)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	2	1.19
(1,610)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	2	1.19
(1,342)	1:13:A:LYS:HA	1:13:A:LYS:HD2	4	1.19
(1,190)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	6	1.19
(1,190)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	6	1.19
(4,18)	1:11:A:TRP:HE3	1:12:A:LEU:HG	1	1.18
(4,18)	1:11:A:TRP:HE3	1:12:A:LEU:HG	2	1.18
(2,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	1	1.18
(2,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	2	1.18
(1,520)	1:1:A:GLU:HA	1:1:A:GLU:HG2	9	1.18
(1,190)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	2	1.18
(1,190)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	2	1.18
(1,190)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	3	1.18
(1,190)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	3	1.18
(1,190)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	4	1.18
(1,190)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	4	1.18
(1,88)	1:9:A:ILE:HB	1:11:A:TRP:H	1	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,18)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	1.17
(2,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	1.17
(1,190)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	7	1.17
(1,190)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	7	1.17
(1,190)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	10	1.17
(1,190)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	10	1.17
(4,18)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	1.16
(2,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	1.16
(1,521)	1:1:A:GLU:HA	1:1:A:GLU:HG3	8	1.16
(1,190)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	1	1.16
(1,190)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	1	1.16
(1,190)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	5	1.16
(1,190)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	5	1.16
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	7	1.15
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	7	1.15
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	7	1.15
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	7	1.15
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	7	1.15
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	7	1.15
(1,571)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	7	1.15
(1,571)	1:24:A:PRO:HG3	1:25:A:CYS:HB2	7	1.15
(1,519)	1:1:A:GLU:HA	1:1:A:GLU:HB3	4	1.15
(1,397)	1:22:A:PRO:HA	1:22:A:PRO:HG3	6	1.15
(3,534)	1:6:A:ARG:HD2	1:7:A:LEU:HG	7	1.14
(3,162)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	7	1.14
(2,566)	1:6:A:ARG:HD2	1:7:A:LEU:HG	7	1.14
(2,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	7	1.14
(1,397)	1:22:A:PRO:HA	1:22:A:PRO:HG3	7	1.14
(1,190)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	8	1.14
(1,190)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	8	1.14
(1,529)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	10	1.13
(1,342)	1:13:A:LYS:HA	1:13:A:LYS:HD2	5	1.13
(4,18)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	1.12
(4,18)	1:11:A:TRP:HE3	1:12:A:LEU:HG	9	1.12
(4,18)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	1.12
(3,552)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	7	1.12
(3,552)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	7	1.12
(3,552)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	7	1.12
(3,452)	1:3:A:GLU:HA	1:6:A:ARG:HB3	8	1.12
(2,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	7	1.12
(2,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	7	1.12
(2,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	7	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,482)	1:3:A:GLU:HA	1:6:A:ARG:HB3	8	1.12
(2,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	1.12
(2,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	9	1.12
(2,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	1.12
(1,529)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	1	1.12
(1,490)	1:14:A:ASP:HB3	1:19:A:SER:HB2	2	1.12
(1,490)	1:14:A:ASP:HB3	1:19:A:SER:HB2	4	1.12
(1,342)	1:13:A:LYS:HA	1:13:A:LYS:HD2	9	1.12
(1,88)	1:9:A:ILE:HB	1:11:A:TRP:H	9	1.12
(4,18)	1:11:A:TRP:HE3	1:12:A:LEU:HG	5	1.11
(3,552)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	2	1.11
(3,552)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	2	1.11
(3,552)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	2	1.11
(3,124)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	1	1.11
(2,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	2	1.11
(2,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	2	1.11
(2,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	2	1.11
(2,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	5	1.11
(2,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	1	1.11
(1,521)	1:1:A:GLU:HA	1:1:A:GLU:HG3	10	1.11
(1,519)	1:1:A:GLU:HA	1:1:A:GLU:HB3	7	1.11
(1,487)	1:8:A:TYR:HA	1:24:A:PRO:HD2	10	1.11
(1,362)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	7	1.11
(1,190)	1:8:A:TYR:HD1	1:9:A:ILE:HG13	9	1.11
(1,190)	1:8:A:TYR:HD2	1:9:A:ILE:HG13	9	1.11
(3,552)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	3	1.1
(3,552)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	3	1.1
(3,552)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	3	1.1
(2,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	3	1.1
(2,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	3	1.1
(2,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	3	1.1
(1,487)	1:8:A:TYR:HA	1:24:A:PRO:HD2	4	1.1
(1,473)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	4	1.1
(1,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	10	1.1
(1,362)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	3	1.1
(1,362)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	5	1.1
(1,362)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	6	1.1
(1,362)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	8	1.1
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	4	1.09
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	4	1.09
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	4	1.09
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	4	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	4	1.09
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	4	1.09
(3,552)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	1	1.09
(3,552)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	1	1.09
(3,552)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	1	1.09
(3,552)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	6	1.09
(3,552)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	6	1.09
(3,552)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	6	1.09
(3,552)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	8	1.09
(3,552)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	8	1.09
(3,552)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	8	1.09
(3,552)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	10	1.09
(3,552)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	10	1.09
(3,552)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	10	1.09
(2,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	1	1.09
(2,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	1	1.09
(2,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	1	1.09
(2,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	6	1.09
(2,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	6	1.09
(2,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	6	1.09
(2,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	8	1.09
(2,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	8	1.09
(2,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	8	1.09
(2,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	10	1.09
(2,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	10	1.09
(2,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	10	1.09
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	4	1.09
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	4	1.09
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	4	1.09
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	4	1.09
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	4	1.09
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	4	1.09
(1,362)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	1	1.09
(1,362)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	4	1.09
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	10	1.08
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	10	1.08
(3,432)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	10	1.08
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	10	1.08
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	10	1.08
(2,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	10	1.08
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	4	1.08
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	4	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	4	1.08
(1,362)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	2	1.08
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	7	1.07
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	7	1.07
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	7	1.07
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	7	1.07
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	7	1.07
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	7	1.07
(3,454)	1:4:A:CYS:HA	1:7:A:LEU:HB3	6	1.07
(2,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	6	1.07
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	7	1.07
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	7	1.07
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	7	1.07
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	7	1.07
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	7	1.07
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	7	1.07
(1,558)	1:2:A:GLU:HA	1:5:A:VAL:HB	3	1.07
(1,490)	1:14:A:ASP:HB3	1:19:A:SER:HB2	10	1.07
(1,487)	1:8:A:TYR:HA	1:24:A:PRO:HD2	3	1.07
(1,487)	1:8:A:TYR:HA	1:24:A:PRO:HD2	8	1.07
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	2	1.06
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	2	1.06
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	2	1.06
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	2	1.06
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	2	1.06
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	2	1.06
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	9	1.06
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	9	1.06
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	9	1.06
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	9	1.06
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	9	1.06
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	9	1.06
(3,162)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	6	1.06
(2,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	6	1.06
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	2	1.06
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	2	1.06
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	2	1.06
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	2	1.06
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	2	1.06
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	2	1.06
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	9	1.06
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	9	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	9	1.06
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	9	1.06
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	9	1.06
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	9	1.06
(1,487)	1:8:A:TYR:HA	1:24:A:PRO:HD2	2	1.06
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD21	9	1.06
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD22	9	1.06
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD23	9	1.06
(1,88)	1:9:A:ILE:HB	1:11:A:TRP:H	4	1.06
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	5	1.05
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	5	1.05
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	5	1.05
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	5	1.05
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	5	1.05
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	5	1.05
(3,552)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	4	1.05
(3,552)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	4	1.05
(3,552)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	4	1.05
(3,454)	1:4:A:CYS:HA	1:7:A:LEU:HB3	1	1.05
(2,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	4	1.05
(2,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	4	1.05
(2,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	4	1.05
(2,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	1	1.05
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	5	1.05
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	5	1.05
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	5	1.05
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	5	1.05
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	5	1.05
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	5	1.05
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	8	1.05
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	8	1.05
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	8	1.05
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD21	2	1.05
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD22	2	1.05
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD23	2	1.05
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD21	7	1.05
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD22	7	1.05
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD23	7	1.05
(1,88)	1:9:A:ILE:HB	1:11:A:TRP:H	7	1.05
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	1	1.04
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	1	1.04
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	1	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	1	1.04
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	1	1.04
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	1	1.04
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	1.04
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	1.04
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	1.04
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	1.04
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	1.04
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	1.04
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	1	1.04
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	1	1.04
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	1	1.04
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	1	1.04
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	1	1.04
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	1	1.04
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	1.04
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	1.04
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	1.04
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	1.04
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	1.04
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	1.04
(1,609)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	9	1.04
(1,609)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	9	1.04
(1,609)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	9	1.04
(1,590)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	10	1.04
(1,590)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	10	1.04
(1,590)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	10	1.04
(1,473)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	1	1.04
(1,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	2	1.04
(1,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	9	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD21	1	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD22	1	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD23	1	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD21	4	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD22	4	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD23	4	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD21	5	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD22	5	1.04
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD23	5	1.04
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	8	1.03
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	8	1.03
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	8	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	8	1.03
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	8	1.03
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	8	1.03
(3,552)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	5	1.03
(3,552)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	5	1.03
(3,552)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	5	1.03
(3,552)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	9	1.03
(3,552)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	9	1.03
(3,552)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	9	1.03
(2,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	5	1.03
(2,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	5	1.03
(2,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	5	1.03
(2,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	9	1.03
(2,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	9	1.03
(2,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	9	1.03
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	8	1.03
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	8	1.03
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	8	1.03
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	8	1.03
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	8	1.03
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	8	1.03
(1,519)	1:1:A:GLU:HA	1:1:A:GLU:HB3	6	1.03
(1,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	7	1.03
(1,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	8	1.03
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG2	8	1.03
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG3	8	1.03
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	3	1.02
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	3	1.02
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	3	1.02
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	3	1.02
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	3	1.02
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	3	1.02
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	3	1.02
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	3	1.02
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	3	1.02
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	3	1.02
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	3	1.02
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	3	1.02
(1,609)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	8	1.02
(1,609)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	8	1.02
(1,609)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	8	1.02
(1,487)	1:8:A:TYR:HA	1:24:A:PRO:HD2	1	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:13:A:LYS:HA	1:13:A:LYS:HD2	10	1.02
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD21	8	1.02
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD22	8	1.02
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD23	8	1.02
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD21	10	1.02
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD22	10	1.02
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD23	10	1.02
(3,548)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	7	1.01
(2,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	7	1.01
(1,473)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	5	1.01
(1,473)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	9	1.01
(1,342)	1:13:A:LYS:HA	1:13:A:LYS:HD2	2	1.01
(1,609)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	1	1.0
(1,609)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	1	1.0
(1,609)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	1	1.0
(1,487)	1:8:A:TYR:HA	1:24:A:PRO:HD2	7	1.0
(1,487)	1:8:A:TYR:HA	1:24:A:PRO:HD2	9	1.0
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	4	1.0
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	4	1.0
(1,423)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	3	1.0
(1,423)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	10	1.0
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD21	3	1.0
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD22	3	1.0
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD23	3	1.0
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	6	0.99
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	6	0.99
(4,15)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	6	0.99
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	6	0.99
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	6	0.99
(4,15)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	6	0.99
(3,444)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	6	0.99
(2,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	6	0.99
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	6	0.99
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	6	0.99
(2,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	6	0.99
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	6	0.99
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	6	0.99
(2,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	6	0.99
(1,519)	1:1:A:GLU:HA	1:1:A:GLU:HB3	1	0.99
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG2	7	0.99
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG3	7	0.99
(1,473)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	2	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	2	0.99
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	2	0.99
(1,423)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	8	0.99
(1,342)	1:13:A:LYS:HA	1:13:A:LYS:HD2	1	0.99
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD21	6	0.99
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD22	6	0.99
(1,227)	1:12:A:LEU:H	1:12:A:LEU:HD23	6	0.99
(1,519)	1:1:A:GLU:HA	1:1:A:GLU:HB3	8	0.98
(1,519)	1:1:A:GLU:HA	1:1:A:GLU:HB3	10	0.98
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG2	1	0.98
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG3	1	0.98
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG2	6	0.98
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG3	6	0.98
(1,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	4	0.98
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG2	3	0.98
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG3	3	0.98
(3,444)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	7	0.97
(3,142)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	9	0.97
(2,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	7	0.97
(2,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	9	0.97
(1,609)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	10	0.97
(1,609)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	10	0.97
(1,609)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	10	0.97
(1,575)	1:2:A:GLU:HB2	1:6:A:ARG:HA	2	0.97
(1,487)	1:8:A:TYR:HA	1:24:A:PRO:HD2	5	0.97
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG2	4	0.97
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG3	4	0.97
(1,276)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	10	0.97
(3,161)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	7	0.96
(2,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	7	0.96
(1,609)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	6	0.96
(1,609)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	6	0.96
(1,609)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	6	0.96
(1,480)	1:8:A:TYR:HA	1:24:A:PRO:HG3	5	0.96
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG2	4	0.96
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG3	4	0.96
(4,7)	1:12:A:LEU:H	1:12:A:LEU:HG	6	0.95
(4,7)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.95
(3,161)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	6	0.95
(3,125)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	7	0.95
(2,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	6	0.95
(2,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	7	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,97)	1:12:A:LEU:H	1:12:A:LEU:HG	6	0.95
(2,97)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.95
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG2	3	0.95
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG3	3	0.95
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG2	5	0.95
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG3	5	0.95
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG2	9	0.95
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG3	9	0.95
(1,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	3	0.95
(1,425)	1:11:A:TRP:HD1	1:23:A:PRO:HD2	5	0.95
(1,342)	1:13:A:LYS:HA	1:13:A:LYS:HD2	3	0.95
(4,7)	1:12:A:LEU:H	1:12:A:LEU:HG	7	0.94
(4,7)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.94
(2,97)	1:12:A:LEU:H	1:12:A:LEU:HG	7	0.94
(2,97)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.94
(1,609)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	7	0.94
(1,609)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	7	0.94
(1,609)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	7	0.94
(1,519)	1:1:A:GLU:HA	1:1:A:GLU:HB3	2	0.94
(1,490)	1:14:A:ASP:HB3	1:19:A:SER:HB2	1	0.94
(1,480)	1:8:A:TYR:HA	1:24:A:PRO:HG3	6	0.94
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG2	2	0.94
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG3	2	0.94
(1,476)	1:9:A:ILE:HA	1:12:A:LEU:HG	2	0.94
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	5	0.94
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	5	0.94
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	8	0.94
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	8	0.94
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	10	0.94
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	10	0.94
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG2	10	0.94
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG3	10	0.94
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD21	4	0.94
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD22	4	0.94
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD23	4	0.94
(1,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	0.94
(1,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	0.94
(1,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	0.94
(1,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	0.94
(4,7)	1:12:A:LEU:H	1:12:A:LEU:HG	3	0.93
(4,7)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.93
(2,97)	1:12:A:LEU:H	1:12:A:LEU:HG	3	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,97)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.93
(1,609)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	5	0.93
(1,609)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	5	0.93
(1,609)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	5	0.93
(1,566)	1:6:A:ARG:HD2	1:7:A:LEU:HG	1	0.93
(1,566)	1:6:A:ARG:HD2	1:7:A:LEU:HG	10	0.93
(1,480)	1:8:A:TYR:HA	1:24:A:PRO:HG3	1	0.93
(1,480)	1:8:A:TYR:HA	1:24:A:PRO:HG3	9	0.93
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG2	10	0.93
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG3	10	0.93
(1,476)	1:9:A:ILE:HA	1:12:A:LEU:HG	4	0.93
(1,423)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	1	0.93
(1,423)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	4	0.93
(1,423)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	5	0.93
(1,342)	1:13:A:LYS:HA	1:13:A:LYS:HD2	7	0.93
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD21	1	0.93
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD22	1	0.93
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD23	1	0.93
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD21	3	0.93
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD22	3	0.93
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD23	3	0.93
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD21	6	0.93
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD22	6	0.93
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD23	6	0.93
(1,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	0.93
(1,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	0.93
(1,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	0.93
(1,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	0.93
(3,161)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	5	0.92
(2,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	5	0.92
(1,575)	1:2:A:GLU:HB2	1:6:A:ARG:HA	8	0.92
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	3	0.92
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	3	0.92
(1,423)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	2	0.92
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	6	0.92
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	6	0.92
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	6	0.92
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	7	0.92
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	7	0.92
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	7	0.92
(1,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	0.92
(1,138)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,7)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.91
(4,7)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.91
(4,7)	1:12:A:LEU:H	1:12:A:LEU:HG	5	0.91
(3,444)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	8	0.91
(3,161)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	9	0.91
(3,138)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	4	0.91
(3,125)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	6	0.91
(2,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	8	0.91
(2,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	9	0.91
(2,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	4	0.91
(2,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	6	0.91
(2,97)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.91
(2,97)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.91
(2,97)	1:12:A:LEU:H	1:12:A:LEU:HG	5	0.91
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD21	2	0.91
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD22	2	0.91
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD23	2	0.91
(1,476)	1:9:A:ILE:HA	1:12:A:LEU:HG	6	0.91
(1,473)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	3	0.91
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	9	0.91
(1,467)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	9	0.91
(1,609)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	3	0.9
(1,609)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	3	0.9
(1,609)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	3	0.9
(1,575)	1:2:A:GLU:HB2	1:6:A:ARG:HA	9	0.9
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG2	8	0.9
(1,479)	1:8:A:TYR:HA	1:24:A:PRO:HG3	8	0.9
(1,476)	1:9:A:ILE:HA	1:12:A:LEU:HG	1	0.9
(1,473)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	10	0.9
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	5	0.9
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	5	0.9
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	5	0.9
(1,342)	1:13:A:LYS:HA	1:13:A:LYS:HD2	8	0.9
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD21	7	0.9
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD22	7	0.9
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD23	7	0.9
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD21	8	0.9
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD22	8	0.9
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD23	8	0.9
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	1	0.9
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	1	0.9
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	1	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,101)	1:24:A:PRO:HG2	1:25:A:CYS:H	1	0.9
(3,142)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	1	0.89
(3,138)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	7	0.89
(2,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	1	0.89
(2,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	7	0.89
(1,540)	1:2:A:GLU:HB2	1:6:A:ARG:H	2	0.89
(1,480)	1:8:A:TYR:HA	1:24:A:PRO:HG3	3	0.89
(1,423)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	9	0.89
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD21	2	0.89
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD22	2	0.89
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD23	2	0.89
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD21	5	0.89
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD22	5	0.89
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD23	5	0.89
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	2	0.89
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	2	0.89
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	2	0.89
(3,444)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	4	0.88
(3,138)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	5	0.88
(3,138)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	6	0.88
(3,138)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.88
(2,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	4	0.88
(2,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	5	0.88
(2,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	6	0.88
(2,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.88
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG11	3	0.88
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG12	3	0.88
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG13	3	0.88
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD21	1	0.88
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD22	1	0.88
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD23	1	0.88
(1,480)	1:8:A:TYR:HA	1:24:A:PRO:HG3	2	0.88
(1,476)	1:9:A:ILE:HA	1:12:A:LEU:HG	3	0.88
(1,473)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	8	0.88
(1,397)	1:22:A:PRO:HA	1:22:A:PRO:HG3	8	0.88
(1,274)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	1	0.88
(1,101)	1:24:A:PRO:HG2	1:25:A:CYS:H	9	0.88
(4,7)	1:12:A:LEU:H	1:12:A:LEU:HG	4	0.87
(3,141)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	9	0.87
(3,138)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	2	0.87
(3,138)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	3	0.87
(3,138)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	8	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,138)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	9	0.87
(2,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	9	0.87
(2,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	2	0.87
(2,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	3	0.87
(2,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	8	0.87
(2,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	9	0.87
(2,97)	1:12:A:LEU:H	1:12:A:LEU:HG	4	0.87
(1,605)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	8	0.87
(1,605)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	8	0.87
(1,605)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	8	0.87
(1,559)	1:19:A:SER:HB2	1:21:A:ARG:HB2	3	0.87
(1,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	4	0.87
(1,476)	1:9:A:ILE:HA	1:12:A:LEU:HG	5	0.87
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD21	10	0.87
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD22	10	0.87
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD23	10	0.87
(3,138)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	1	0.86
(2,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	1	0.86
(1,609)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	4	0.86
(1,609)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	4	0.86
(1,609)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	4	0.86
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD21	10	0.86
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD22	10	0.86
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD23	10	0.86
(1,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	8	0.86
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG2	5	0.86
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG3	5	0.86
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	3	0.86
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	3	0.86
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	3	0.86
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	4	0.86
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	4	0.86
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	4	0.86
(1,93)	1:6:A:ARG:HG2	1:7:A:LEU:H	10	0.86
(3,161)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	4	0.85
(2,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	4	0.85
(1,605)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	5	0.85
(1,605)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	5	0.85
(1,605)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	5	0.85
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	2	0.85
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	2	0.85
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	2	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	7	0.85
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	7	0.85
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	7	0.85
(1,519)	1:1:A:GLU:HA	1:1:A:GLU:HB3	9	0.85
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD21	3	0.85
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD22	3	0.85
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD23	3	0.85
(1,476)	1:9:A:ILE:HA	1:12:A:LEU:HG	7	0.85
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD21	9	0.85
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD22	9	0.85
(1,328)	1:12:A:LEU:HA	1:12:A:LEU:HD23	9	0.85
(1,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	4	0.85
(1,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	4	0.85
(3,578)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	6	0.84
(3,578)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	6	0.84
(3,578)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	6	0.84
(3,161)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	8	0.84
(3,139)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	4	0.84
(3,139)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	4	0.84
(3,139)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	7	0.84
(3,139)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	7	0.84
(2,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	6	0.84
(2,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	6	0.84
(2,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	6	0.84
(2,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	8	0.84
(2,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	4	0.84
(2,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	4	0.84
(2,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	7	0.84
(2,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	7	0.84
(1,605)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	9	0.84
(1,605)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	9	0.84
(1,605)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	9	0.84
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD21	4	0.84
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD22	4	0.84
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD23	4	0.84
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD21	5	0.84
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD22	5	0.84
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD23	5	0.84
(1,487)	1:8:A:TYR:HA	1:24:A:PRO:HD2	6	0.84
(1,480)	1:8:A:TYR:HA	1:24:A:PRO:HG3	8	0.84
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG2	9	0.84
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG3	9	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,578)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	0.83
(3,578)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	0.83
(3,578)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	0.83
(3,578)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.83
(3,578)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.83
(3,578)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.83
(3,142)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	5	0.83
(3,132)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.83
(3,132)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.83
(2,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	0.83
(2,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	0.83
(2,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	0.83
(2,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.83
(2,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.83
(2,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.83
(2,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	5	0.83
(2,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.83
(2,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.83
(1,605)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	6	0.83
(1,605)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	6	0.83
(1,605)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	6	0.83
(1,605)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	7	0.83
(1,605)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	7	0.83
(1,605)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	7	0.83
(1,605)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	10	0.83
(1,605)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	10	0.83
(1,605)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	10	0.83
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	4	0.83
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	4	0.83
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	4	0.83
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	10	0.83
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	10	0.83
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	10	0.83
(1,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	7	0.83
(1,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	7	0.83
(1,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	7	0.83
(1,575)	1:2:A:GLU:HB2	1:6:A:ARG:HA	10	0.83
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD21	6	0.83
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD22	6	0.83
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD23	6	0.83
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD21	9	0.83
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD22	9	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD23	9	0.83
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG2	1	0.83
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG3	1	0.83
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG2	2	0.83
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG3	2	0.83
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG2	6	0.83
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG3	6	0.83
(3,578)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	2	0.82
(3,578)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	2	0.82
(3,578)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	2	0.82
(3,444)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	3	0.82
(3,161)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	2	0.82
(3,132)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.82
(3,132)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.82
(3,132)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.82
(3,132)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.82
(3,132)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.82
(3,132)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.82
(3,132)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.82
(3,132)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.82
(2,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	2	0.82
(2,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	2	0.82
(2,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	2	0.82
(2,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	3	0.82
(2,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	2	0.82
(2,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.82
(2,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.82
(2,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.82
(2,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.82
(2,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.82
(2,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.82
(2,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.82
(2,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.82
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	1	0.82
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	1	0.82
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	1	0.82
(1,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	2	0.82
(1,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	2	0.82
(1,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	2	0.82
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD21	8	0.82
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD22	8	0.82
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD23	8	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,476)	1:9:A:ILE:HA	1:12:A:LEU:HG	10	0.82
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	2	0.82
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	2	0.82
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	3	0.82
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	3	0.82
(3,444)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	1	0.81
(3,142)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	7	0.81
(3,139)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	10	0.81
(3,139)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	10	0.81
(3,43)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.81
(3,43)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.81
(3,43)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.81
(3,43)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.81
(2,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	1	0.81
(2,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	7	0.81
(2,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	10	0.81
(2,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	10	0.81
(2,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.81
(2,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.81
(2,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.81
(2,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.81
(1,609)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	2	0.81
(1,609)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	2	0.81
(1,609)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	2	0.81
(1,605)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	1	0.81
(1,605)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	1	0.81
(1,605)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	1	0.81
(1,605)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	3	0.81
(1,605)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	3	0.81
(1,605)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	3	0.81
(1,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	1	0.81
(1,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	1	0.81
(1,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	1	0.81
(1,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	3	0.81
(1,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	3	0.81
(1,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	3	0.81
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD21	7	0.81
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD22	7	0.81
(1,514)	1:9:A:ILE:HA	1:12:A:LEU:HD23	7	0.81
(1,397)	1:22:A:PRO:HA	1:22:A:PRO:HG3	4	0.81
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	5	0.81
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	5	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:6:A:ARG:HA	1:6:A:ARG:HG2	8	0.81
(1,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	8	0.81
(1,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	8	0.81
(1,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	3	0.81
(1,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	5	0.81
(3,444)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	10	0.8
(3,417)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	1	0.8
(3,417)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	5	0.8
(3,417)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	6	0.8
(3,142)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	2	0.8
(3,139)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	2	0.8
(3,139)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	2	0.8
(3,139)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	6	0.8
(3,139)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	6	0.8
(3,139)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	9	0.8
(3,139)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	9	0.8
(3,43)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.8
(3,43)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.8
(2,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	10	0.8
(2,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	1	0.8
(2,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	5	0.8
(2,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	6	0.8
(2,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	2	0.8
(2,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	2	0.8
(2,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	2	0.8
(2,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	6	0.8
(2,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	6	0.8
(2,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	9	0.8
(2,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	9	0.8
(2,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.8
(2,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.8
(1,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	6	0.8
(1,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	6	0.8
(1,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	6	0.8
(1,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	8	0.8
(1,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	8	0.8
(1,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	8	0.8
(1,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	10	0.8
(1,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	10	0.8
(1,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	10	0.8
(1,480)	1:8:A:TYR:HA	1:24:A:PRO:HG3	4	0.8
(1,270)	1:6:A:ARG:HA	1:6:A:ARG:HG2	2	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:6:A:ARG:HA	1:6:A:ARG:HG2	4	0.8
(1,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	7	0.8
(1,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	7	0.8
(1,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	4	0.8
(1,101)	1:24:A:PRO:HG2	1:25:A:CYS:H	6	0.8
(3,578)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	9	0.79
(3,578)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	9	0.79
(3,578)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	9	0.79
(3,139)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	1	0.79
(3,139)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	1	0.79
(2,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	9	0.79
(2,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	9	0.79
(2,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	9	0.79
(2,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	1	0.79
(2,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	1	0.79
(1,605)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	2	0.79
(1,605)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	2	0.79
(1,605)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	2	0.79
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD11	6	0.79
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD12	6	0.79
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD13	6	0.79
(1,476)	1:9:A:ILE:HA	1:12:A:LEU:HG	8	0.79
(1,398)	1:22:A:PRO:HA	1:22:A:PRO:HB3	4	0.79
(1,398)	1:22:A:PRO:HA	1:22:A:PRO:HB3	8	0.79
(4,31)	1:11:A:TRP:HE3	1:12:A:LEU:HG	7	0.78
(3,417)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	2	0.78
(3,417)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	7	0.78
(3,417)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	8	0.78
(3,417)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.78
(3,139)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	5	0.78
(3,139)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	5	0.78
(3,139)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	8	0.78
(3,139)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	8	0.78
(2,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	7	0.78
(2,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	2	0.78
(2,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	7	0.78
(2,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	8	0.78
(2,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.78
(2,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	5	0.78
(2,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	5	0.78
(2,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	8	0.78
(2,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	8	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	1	0.78
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	1	0.78
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	1	0.78
(1,423)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	6	0.78
(1,398)	1:22:A:PRO:HA	1:22:A:PRO:HB3	1	0.78
(1,398)	1:22:A:PRO:HA	1:22:A:PRO:HB3	3	0.78
(1,398)	1:22:A:PRO:HA	1:22:A:PRO:HB3	6	0.78
(1,398)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.78
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG2	7	0.78
(1,382)	1:21:A:ARG:HA	1:21:A:ARG:HG3	7	0.78
(1,273)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	6	0.78
(1,270)	1:6:A:ARG:HA	1:6:A:ARG:HG2	3	0.78
(1,270)	1:6:A:ARG:HA	1:6:A:ARG:HG2	5	0.78
(1,267)	1:6:A:ARG:HA	1:6:A:ARG:HD3	6	0.78
(1,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	2	0.78
(1,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	2	0.78
(1,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	6	0.78
(1,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	6	0.78
(1,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.78
(1,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.78
(1,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	2	0.78
(1,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	6	0.78
(1,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	8	0.78
(4,31)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	0.77
(3,444)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	9	0.77
(3,417)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	3	0.77
(3,417)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	9	0.77
(3,161)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	3	0.77
(3,141)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	1	0.77
(3,43)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.77
(3,43)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.77
(3,43)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.77
(2,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	0.77
(2,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	9	0.77
(2,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	3	0.77
(2,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	9	0.77
(2,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	3	0.77
(2,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	1	0.77
(2,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.77
(2,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.77
(2,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.77
(1,581)	1:1:A:GLU:HB3	1:2:A:GLU:HG2	9	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	10	0.77
(1,398)	1:22:A:PRO:HA	1:22:A:PRO:HB3	7	0.77
(1,267)	1:6:A:ARG:HA	1:6:A:ARG:HD3	3	0.77
(1,199)	1:24:A:PRO:HD2	1:25:A:CYS:H	8	0.77
(1,181)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	3	0.77
(1,181)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	8	0.77
(1,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	0.77
(1,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	0.77
(4,31)	1:11:A:TRP:HE3	1:12:A:LEU:HG	1	0.76
(4,31)	1:11:A:TRP:HE3	1:12:A:LEU:HG	2	0.76
(3,417)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	4	0.76
(2,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	1	0.76
(2,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	2	0.76
(2,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	4	0.76
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	9	0.76
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	9	0.76
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	9	0.76
(1,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	4	0.76
(1,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	4	0.76
(1,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	4	0.76
(1,342)	1:13:A:LYS:HA	1:13:A:LYS:HD2	6	0.76
(1,276)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	7	0.76
(1,199)	1:24:A:PRO:HD2	1:25:A:CYS:H	4	0.76
(1,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	5	0.76
(1,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	5	0.76
(1,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	9	0.76
(4,31)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	0.75
(3,578)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	7	0.75
(3,578)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	7	0.75
(3,578)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	7	0.75
(3,444)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	2	0.75
(3,444)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	5	0.75
(3,162)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	9	0.75
(3,142)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	4	0.75
(3,139)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	3	0.75
(3,139)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	3	0.75
(2,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	7	0.75
(2,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	7	0.75
(2,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	7	0.75
(2,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	0.75
(2,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	2	0.75
(2,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	9	0.75
(2,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	4	0.75
(2,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	3	0.75
(2,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	3	0.75
(1,605)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	4	0.75
(1,605)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	4	0.75
(1,605)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	4	0.75
(1,581)	1:1:A:GLU:HB3	1:2:A:GLU:HG2	2	0.75
(1,555)	1:2:A:GLU:HA	1:5:A:VAL:HG21	6	0.75
(1,555)	1:2:A:GLU:HA	1:5:A:VAL:HG22	6	0.75
(1,555)	1:2:A:GLU:HA	1:5:A:VAL:HG23	6	0.75
(1,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	5	0.75
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	2	0.75
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	2	0.75
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	2	0.75
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	4	0.75
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	4	0.75
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	4	0.75
(1,270)	1:6:A:ARG:HA	1:6:A:ARG:HG2	6	0.75
(1,199)	1:24:A:PRO:HD2	1:25:A:CYS:H	10	0.75
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	8	0.75
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	8	0.75
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	8	0.75
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	10	0.75
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	10	0.75
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	10	0.75
(1,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	1	0.75
(1,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	1	0.75
(1,153)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	3	0.75
(1,153)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	3	0.75
(1,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	7	0.75
(1,123)	1:23:A:PRO:HB2	1:25:A:CYS:H	7	0.75
(4,31)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	0.74
(3,578)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	5	0.74
(3,578)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	5	0.74
(3,578)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	5	0.74
(2,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	5	0.74
(2,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	5	0.74
(2,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	5	0.74
(2,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	0.74
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	1	0.74
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	1	0.74
(1,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	5	0.74
(1,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	5	0.74
(1,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	5	0.74
(1,586)	1:12:A:LEU:HD11	1:24:A:PRO:HD3	9	0.74
(1,586)	1:12:A:LEU:HD12	1:24:A:PRO:HD3	9	0.74
(1,586)	1:12:A:LEU:HD13	1:24:A:PRO:HD3	9	0.74
(1,540)	1:2:A:GLU:HB2	1:6:A:ARG:H	9	0.74
(1,494)	1:22:A:PRO:HA	1:23:A:PRO:HD2	2	0.74
(1,494)	1:22:A:PRO:HA	1:23:A:PRO:HD2	9	0.74
(1,397)	1:22:A:PRO:HA	1:22:A:PRO:HG3	3	0.74
(1,360)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.74
(1,322)	1:11:A:TRP:HA	1:11:A:TRP:HB2	1	0.74
(1,322)	1:11:A:TRP:HA	1:11:A:TRP:HB2	2	0.74
(1,322)	1:11:A:TRP:HA	1:11:A:TRP:HB2	4	0.74
(1,322)	1:11:A:TRP:HA	1:11:A:TRP:HB2	6	0.74
(1,322)	1:11:A:TRP:HA	1:11:A:TRP:HB2	7	0.74
(1,199)	1:24:A:PRO:HD2	1:25:A:CYS:H	7	0.74
(1,181)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	4	0.74
(3,530)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	4	0.73
(3,142)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	8	0.73
(3,86)	1:7:A:LEU:H	1:7:A:LEU:HB3	10	0.73
(3,43)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.73
(2,562)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	4	0.73
(2,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	8	0.73
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	10	0.73
(2,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.73
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	8	0.73
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	8	0.73
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	8	0.73
(1,398)	1:22:A:PRO:HA	1:22:A:PRO:HB3	2	0.73
(1,398)	1:22:A:PRO:HA	1:22:A:PRO:HB3	5	0.73
(1,398)	1:22:A:PRO:HA	1:22:A:PRO:HB3	9	0.73
(1,360)	1:17:A:PRO:HA	1:17:A:PRO:HB3	9	0.73
(1,322)	1:11:A:TRP:HA	1:11:A:TRP:HB2	3	0.73
(1,274)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	7	0.73
(1,267)	1:6:A:ARG:HA	1:6:A:ARG:HD3	5	0.73
(1,199)	1:24:A:PRO:HD2	1:25:A:CYS:H	9	0.73
(1,181)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.73
(3,162)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	5	0.72
(3,86)	1:7:A:LEU:H	1:7:A:LEU:HB3	2	0.72
(3,86)	1:7:A:LEU:H	1:7:A:LEU:HB3	7	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	5	0.72
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	2	0.72
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	7	0.72
(1,580)	1:11:A:TRP:HB2	1:21:A:ARG:HD2	3	0.72
(1,556)	1:2:A:GLU:HA	1:5:A:VAL:HG11	6	0.72
(1,556)	1:2:A:GLU:HA	1:5:A:VAL:HG12	6	0.72
(1,556)	1:2:A:GLU:HA	1:5:A:VAL:HG13	6	0.72
(1,494)	1:22:A:PRO:HA	1:23:A:PRO:HD2	8	0.72
(1,476)	1:9:A:ILE:HA	1:12:A:LEU:HG	9	0.72
(1,466)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	2	0.72
(1,466)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	9	0.72
(1,423)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	7	0.72
(1,322)	1:11:A:TRP:HA	1:11:A:TRP:HB2	10	0.72
(1,273)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	5	0.72
(3,86)	1:7:A:LEU:H	1:7:A:LEU:HB3	1	0.71
(3,86)	1:7:A:LEU:H	1:7:A:LEU:HB3	4	0.71
(3,86)	1:7:A:LEU:H	1:7:A:LEU:HB3	5	0.71
(3,86)	1:7:A:LEU:H	1:7:A:LEU:HB3	6	0.71
(3,86)	1:7:A:LEU:H	1:7:A:LEU:HB3	8	0.71
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	1	0.71
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	4	0.71
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	5	0.71
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	6	0.71
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	8	0.71
(1,554)	1:4:A:CYS:HA	1:7:A:LEU:HG	6	0.71
(1,494)	1:22:A:PRO:HA	1:23:A:PRO:HD2	4	0.71
(1,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	9	0.71
(1,456)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	9	0.71
(1,397)	1:22:A:PRO:HA	1:22:A:PRO:HG3	10	0.71
(1,322)	1:11:A:TRP:HA	1:11:A:TRP:HB2	5	0.71
(1,322)	1:11:A:TRP:HA	1:11:A:TRP:HB2	8	0.71
(1,322)	1:11:A:TRP:HA	1:11:A:TRP:HB2	9	0.71
(1,313)	1:10:A:GLN:HA	1:10:A:GLN:HG3	4	0.71
(1,273)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	8	0.71
(1,199)	1:24:A:PRO:HD2	1:25:A:CYS:H	2	0.71
(1,101)	1:24:A:PRO:HG2	1:25:A:CYS:H	5	0.71
(4,31)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.7
(4,31)	1:11:A:TRP:HE3	1:12:A:LEU:HG	9	0.7
(4,31)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.7
(3,86)	1:7:A:LEU:H	1:7:A:LEU:HB3	3	0.7
(3,86)	1:7:A:LEU:H	1:7:A:LEU:HB3	9	0.7
(2,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	9	0.7
(2,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.7
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	3	0.7
(2,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	9	0.7
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	6	0.7
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	6	0.7
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	6	0.7
(1,494)	1:22:A:PRO:HA	1:23:A:PRO:HD2	1	0.7
(1,494)	1:22:A:PRO:HA	1:23:A:PRO:HD2	3	0.7
(1,494)	1:22:A:PRO:HA	1:23:A:PRO:HD2	5	0.7
(1,480)	1:8:A:TYR:HA	1:24:A:PRO:HG3	10	0.7
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	5	0.7
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	5	0.7
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	5	0.7
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	9	0.7
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	9	0.7
(1,171)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	9	0.7
(1,101)	1:24:A:PRO:HG2	1:25:A:CYS:H	4	0.7
(1,101)	1:24:A:PRO:HG2	1:25:A:CYS:H	8	0.7
(1,54)	1:18:A:SER:H	1:18:A:SER:HB3	6	0.7
(4,31)	1:11:A:TRP:HE3	1:12:A:LEU:HG	5	0.69
(3,162)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	2	0.69
(3,162)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	4	0.69
(3,160)	1:23:A:PRO:HB3	1:25:A:CYS:H	6	0.69
(3,142)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	3	0.69
(3,142)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	6	0.69
(2,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	5	0.69
(2,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	2	0.69
(2,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	4	0.69
(2,177)	1:23:A:PRO:HB3	1:25:A:CYS:H	6	0.69
(2,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	3	0.69
(2,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	6	0.69
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD11	5	0.69
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD12	5	0.69
(1,592)	1:2:A:GLU:HG3	1:9:A:ILE:HD13	5	0.69
(1,437)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	1	0.69
(1,437)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	3	0.69
(1,437)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.69
(1,273)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	2	0.69
(1,199)	1:24:A:PRO:HD2	1:25:A:CYS:H	3	0.69
(1,90)	1:10:A:GLN:HB3	1:11:A:TRP:H	5	0.69
(1,54)	1:18:A:SER:H	1:18:A:SER:HB3	5	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:18:A:SER:H	1:18:A:SER:HB3	9	0.69
(3,578)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	3	0.68
(3,578)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	3	0.68
(3,578)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	3	0.68
(3,578)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	8	0.68
(3,578)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	8	0.68
(3,578)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	8	0.68
(3,530)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	2	0.68
(3,530)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	9	0.68
(3,530)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	10	0.68
(3,142)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.68
(3,90)	1:12:A:LEU:H	1:12:A:LEU:HB3	9	0.68
(2,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	3	0.68
(2,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	3	0.68
(2,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	3	0.68
(2,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	8	0.68
(2,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	8	0.68
(2,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	8	0.68
(2,562)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	2	0.68
(2,562)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	9	0.68
(2,562)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	10	0.68
(2,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.68
(2,96)	1:12:A:LEU:H	1:12:A:LEU:HB3	9	0.68
(1,575)	1:2:A:GLU:HB2	1:6:A:ARG:HA	3	0.68
(1,554)	1:4:A:CYS:HA	1:7:A:LEU:HG	1	0.68
(1,508)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	6	0.68
(1,508)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	6	0.68
(1,508)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	6	0.68
(1,437)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	2	0.68
(1,437)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	9	0.68
(1,360)	1:17:A:PRO:HA	1:17:A:PRO:HB3	8	0.68
(1,299)	1:9:A:ILE:HA	1:9:A:ILE:HG12	8	0.68
(1,273)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	3	0.68
(1,267)	1:6:A:ARG:HA	1:6:A:ARG:HD3	4	0.68
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG2	8	0.68
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG3	8	0.68
(1,54)	1:18:A:SER:H	1:18:A:SER:HB3	1	0.68
(3,578)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	4	0.67
(3,578)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	4	0.67
(3,578)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	4	0.67
(3,160)	1:23:A:PRO:HB3	1:25:A:CYS:H	5	0.67
(3,141)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	5	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,90)	1:12:A:LEU:H	1:12:A:LEU:HB3	1	0.67
(3,90)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.67
(3,90)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.67
(3,90)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.67
(3,90)	1:12:A:LEU:H	1:12:A:LEU:HB3	5	0.67
(3,90)	1:12:A:LEU:H	1:12:A:LEU:HB3	8	0.67
(3,90)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.67
(2,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	4	0.67
(2,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	4	0.67
(2,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	4	0.67
(2,177)	1:23:A:PRO:HB3	1:25:A:CYS:H	5	0.67
(2,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	5	0.67
(2,96)	1:12:A:LEU:H	1:12:A:LEU:HB3	1	0.67
(2,96)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.67
(2,96)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.67
(2,96)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.67
(2,96)	1:12:A:LEU:H	1:12:A:LEU:HB3	5	0.67
(2,96)	1:12:A:LEU:H	1:12:A:LEU:HB3	8	0.67
(2,96)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.67
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	9	0.67
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	9	0.67
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	9	0.67
(1,456)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	2	0.67
(1,437)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	4	0.67
(1,437)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	5	0.67
(1,437)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	8	0.67
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	6	0.67
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	6	0.67
(1,360)	1:17:A:PRO:HA	1:17:A:PRO:HB3	1	0.67
(1,360)	1:17:A:PRO:HA	1:17:A:PRO:HB3	3	0.67
(1,360)	1:17:A:PRO:HA	1:17:A:PRO:HB3	4	0.67
(1,360)	1:17:A:PRO:HA	1:17:A:PRO:HB3	5	0.67
(1,299)	1:9:A:ILE:HA	1:9:A:ILE:HG12	10	0.67
(3,530)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	5	0.66
(3,90)	1:12:A:LEU:H	1:12:A:LEU:HB3	7	0.66
(2,562)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	5	0.66
(2,96)	1:12:A:LEU:H	1:12:A:LEU:HB3	7	0.66
(1,612)	1:9:A:ILE:HG21	1:12:A:LEU:HB2	9	0.66
(1,612)	1:9:A:ILE:HG22	1:12:A:LEU:HB2	9	0.66
(1,612)	1:9:A:ILE:HG23	1:12:A:LEU:HB2	9	0.66
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	2	0.66
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	2	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	2	0.66
(1,540)	1:2:A:GLU:HB2	1:6:A:ARG:H	10	0.66
(1,456)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	6	0.66
(1,393)	1:22:A:PRO:HA	1:22:A:PRO:HD2	3	0.66
(1,393)	1:22:A:PRO:HA	1:22:A:PRO:HD2	4	0.66
(1,393)	1:22:A:PRO:HA	1:22:A:PRO:HD2	8	0.66
(1,360)	1:17:A:PRO:HA	1:17:A:PRO:HB3	2	0.66
(1,360)	1:17:A:PRO:HA	1:17:A:PRO:HB3	6	0.66
(1,360)	1:17:A:PRO:HA	1:17:A:PRO:HB3	7	0.66
(1,299)	1:9:A:ILE:HA	1:9:A:ILE:HG12	2	0.66
(1,299)	1:9:A:ILE:HA	1:9:A:ILE:HG12	5	0.66
(1,299)	1:9:A:ILE:HA	1:9:A:ILE:HG12	6	0.66
(1,276)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	1	0.66
(1,101)	1:24:A:PRO:HG2	1:25:A:CYS:H	2	0.66
(4,38)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	6	0.65
(3,452)	1:3:A:GLU:HA	1:6:A:ARG:HB3	6	0.65
(3,135)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.65
(3,135)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.65
(3,90)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.65
(2,620)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	6	0.65
(2,482)	1:3:A:GLU:HA	1:6:A:ARG:HB3	6	0.65
(2,145)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.65
(2,145)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.65
(2,96)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.65
(1,581)	1:1:A:GLU:HB3	1:2:A:GLU:HG2	5	0.65
(1,570)	1:24:A:PRO:HB2	1:25:A:CYS:HB2	4	0.65
(1,483)	1:7:A:LEU:HA	1:10:A:GLN:HB3	4	0.65
(1,480)	1:8:A:TYR:HA	1:24:A:PRO:HG3	7	0.65
(1,473)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	7	0.65
(1,437)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	6	0.65
(1,437)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	7	0.65
(1,415)	1:21:A:ARG:HA	1:22:A:PRO:HD3	7	0.65
(1,393)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.65
(1,299)	1:9:A:ILE:HA	1:9:A:ILE:HG12	7	0.65
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG2	3	0.65
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG3	3	0.65
(3,530)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	8	0.64
(3,135)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.64
(3,135)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.64
(3,135)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.64
(2,562)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	8	0.64
(2,145)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,145)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.64
(2,145)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.64
(1,580)	1:11:A:TRP:HB2	1:21:A:ARG:HD2	5	0.64
(1,473)	1:11:A:TRP:HB2	1:24:A:PRO:HD3	6	0.64
(1,456)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	5	0.64
(1,415)	1:21:A:ARG:HA	1:22:A:PRO:HD3	3	0.64
(1,299)	1:9:A:ILE:HA	1:9:A:ILE:HG12	1	0.64
(1,299)	1:9:A:ILE:HA	1:9:A:ILE:HG12	3	0.64
(1,299)	1:9:A:ILE:HA	1:9:A:ILE:HG12	9	0.64
(1,224)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	10	0.64
(1,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	10	0.64
(4,38)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	8	0.63
(3,135)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.63
(3,135)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.63
(3,135)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.63
(3,135)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	0.63
(2,620)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	8	0.63
(2,145)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.63
(2,145)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.63
(2,145)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.63
(2,145)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	0.63
(1,612)	1:9:A:ILE:HG21	1:12:A:LEU:HB2	1	0.63
(1,612)	1:9:A:ILE:HG22	1:12:A:LEU:HB2	1	0.63
(1,612)	1:9:A:ILE:HG23	1:12:A:LEU:HB2	1	0.63
(1,612)	1:9:A:ILE:HG21	1:12:A:LEU:HB2	2	0.63
(1,612)	1:9:A:ILE:HG22	1:12:A:LEU:HB2	2	0.63
(1,612)	1:9:A:ILE:HG23	1:12:A:LEU:HB2	2	0.63
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	3	0.63
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	3	0.63
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	3	0.63
(1,575)	1:2:A:GLU:HB2	1:6:A:ARG:HA	7	0.63
(1,418)	1:23:A:PRO:HA	1:23:A:PRO:HB3	2	0.63
(1,418)	1:23:A:PRO:HA	1:23:A:PRO:HB3	3	0.63
(1,418)	1:23:A:PRO:HA	1:23:A:PRO:HB3	9	0.63
(1,415)	1:21:A:ARG:HA	1:22:A:PRO:HD3	4	0.63
(1,415)	1:21:A:ARG:HA	1:22:A:PRO:HD3	8	0.63
(1,415)	1:21:A:ARG:HA	1:22:A:PRO:HD3	10	0.63
(1,273)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	4	0.63
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG2	4	0.63
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG3	4	0.63
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG2	10	0.63
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG3	10	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:18:A:SER:H	1:18:A:SER:HB2	4	0.63
(4,38)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	5	0.62
(3,530)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	1	0.62
(3,279)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.62
(3,279)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.62
(3,279)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.62
(3,279)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.62
(3,279)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.62
(3,279)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.62
(3,279)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.62
(3,279)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.62
(3,279)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.62
(3,162)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	8	0.62
(3,135)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	0.62
(2,620)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	5	0.62
(2,562)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	1	0.62
(2,305)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.62
(2,305)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.62
(2,305)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.62
(2,305)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.62
(2,305)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.62
(2,305)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.62
(2,305)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.62
(2,305)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.62
(2,305)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.62
(2,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	8	0.62
(2,145)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	0.62
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG11	5	0.62
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG12	5	0.62
(1,587)	1:2:A:GLU:HG3	1:5:A:VAL:HG13	5	0.62
(1,581)	1:1:A:GLU:HB3	1:2:A:GLU:HG2	8	0.62
(1,575)	1:2:A:GLU:HB2	1:6:A:ARG:HA	4	0.62
(1,575)	1:2:A:GLU:HB2	1:6:A:ARG:HA	5	0.62
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB2	8	0.62
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB3	8	0.62
(1,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	2	0.62
(1,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	3	0.62
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	8	0.62
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	8	0.62
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	8	0.62
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	9	0.62
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	9	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	9	0.62
(1,456)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	4	0.62
(1,456)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	8	0.62
(1,418)	1:23:A:PRO:HA	1:23:A:PRO:HB3	4	0.62
(1,418)	1:23:A:PRO:HA	1:23:A:PRO:HB3	5	0.62
(1,418)	1:23:A:PRO:HA	1:23:A:PRO:HB3	8	0.62
(1,418)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.62
(1,415)	1:21:A:ARG:HA	1:22:A:PRO:HD3	6	0.62
(1,393)	1:22:A:PRO:HA	1:22:A:PRO:HD2	7	0.62
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	8	0.62
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	8	0.62
(1,313)	1:10:A:GLN:HA	1:10:A:GLN:HG3	7	0.62
(1,267)	1:6:A:ARG:HA	1:6:A:ARG:HD3	8	0.62
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG2	1	0.62
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG3	1	0.62
(1,224)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	4	0.62
(1,199)	1:24:A:PRO:HD2	1:25:A:CYS:H	1	0.62
(4,2)	1:6:A:ARG:H	1:6:A:ARG:HG2	1	0.61
(3,530)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	3	0.61
(3,452)	1:3:A:GLU:HA	1:6:A:ARG:HB3	1	0.61
(3,279)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.61
(3,141)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	2	0.61
(3,125)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	4	0.61
(2,562)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	3	0.61
(2,482)	1:3:A:GLU:HA	1:6:A:ARG:HB3	1	0.61
(2,305)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.61
(2,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	2	0.61
(2,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	4	0.61
(2,15)	1:6:A:ARG:H	1:6:A:ARG:HG2	1	0.61
(1,612)	1:9:A:ILE:HG21	1:12:A:LEU:HB2	4	0.61
(1,612)	1:9:A:ILE:HG22	1:12:A:LEU:HB2	4	0.61
(1,612)	1:9:A:ILE:HG23	1:12:A:LEU:HB2	4	0.61
(1,581)	1:1:A:GLU:HB3	1:2:A:GLU:HG2	1	0.61
(1,510)	1:12:A:LEU:HA	1:16:A:GLY:HA3	1	0.61
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB2	3	0.61
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB3	3	0.61
(1,418)	1:23:A:PRO:HA	1:23:A:PRO:HB3	1	0.61
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	1	0.61
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	1	0.61
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	9	0.61
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	9	0.61
(1,313)	1:10:A:GLN:HA	1:10:A:GLN:HG3	9	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG2	2	0.61
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG3	2	0.61
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG2	9	0.61
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG3	9	0.61
(1,90)	1:10:A:GLN:HB3	1:11:A:TRP:H	10	0.61
(4,38)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	1	0.6
(4,38)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	2	0.6
(4,38)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	3	0.6
(4,38)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	10	0.6
(4,2)	1:6:A:ARG:H	1:6:A:ARG:HG2	7	0.6
(3,452)	1:3:A:GLU:HA	1:6:A:ARG:HB3	5	0.6
(3,141)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	8	0.6
(3,125)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	2	0.6
(2,620)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	1	0.6
(2,620)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	2	0.6
(2,620)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	3	0.6
(2,620)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	10	0.6
(2,482)	1:3:A:GLU:HA	1:6:A:ARG:HB3	5	0.6
(2,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	8	0.6
(2,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	2	0.6
(2,15)	1:6:A:ARG:H	1:6:A:ARG:HG2	7	0.6
(1,612)	1:9:A:ILE:HG21	1:12:A:LEU:HB2	3	0.6
(1,612)	1:9:A:ILE:HG22	1:12:A:LEU:HB2	3	0.6
(1,612)	1:9:A:ILE:HG23	1:12:A:LEU:HB2	3	0.6
(1,566)	1:6:A:ARG:HD2	1:7:A:LEU:HG	7	0.6
(1,518)	1:1:A:GLU:HA	1:1:A:GLU:HB2	3	0.6
(1,494)	1:22:A:PRO:HA	1:23:A:PRO:HD2	10	0.6
(1,418)	1:23:A:PRO:HA	1:23:A:PRO:HB3	6	0.6
(1,418)	1:23:A:PRO:HA	1:23:A:PRO:HB3	7	0.6
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	4	0.6
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	4	0.6
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	7	0.6
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	7	0.6
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG2	6	0.6
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG3	6	0.6
(1,275)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	9	0.6
(1,266)	1:6:A:ARG:HA	1:6:A:ARG:HD2	9	0.6
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG2	7	0.6
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG3	7	0.6
(1,123)	1:23:A:PRO:HB2	1:25:A:CYS:H	2	0.6
(1,101)	1:24:A:PRO:HG2	1:25:A:CYS:H	3	0.6
(1,53)	1:18:A:SER:H	1:18:A:SER:HB2	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,530)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	7	0.59
(2,562)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	7	0.59
(1,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	4	0.59
(1,508)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	7	0.59
(1,508)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	7	0.59
(1,508)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	7	0.59
(1,483)	1:7:A:LEU:HA	1:10:A:GLN:HB3	9	0.59
(1,397)	1:22:A:PRO:HA	1:22:A:PRO:HG3	1	0.59
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	10	0.59
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	10	0.59
(1,354)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	2	0.59
(1,354)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	3	0.59
(1,354)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	4	0.59
(1,354)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	5	0.59
(1,354)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	6	0.59
(1,354)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	7	0.59
(1,354)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	8	0.59
(1,313)	1:10:A:GLN:HA	1:10:A:GLN:HG3	1	0.59
(1,299)	1:9:A:ILE:HA	1:9:A:ILE:HG12	4	0.59
(1,267)	1:6:A:ARG:HA	1:6:A:ARG:HD3	2	0.59
(1,224)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	6	0.59
(1,224)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	7	0.59
(1,224)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	8	0.59
(1,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	7	0.59
(1,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	7	0.59
(1,53)	1:18:A:SER:H	1:18:A:SER:HB2	2	0.59
(3,125)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	5	0.58
(3,125)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	9	0.58
(2,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	5	0.58
(2,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	9	0.58
(1,483)	1:7:A:LEU:HA	1:10:A:GLN:HB3	7	0.58
(1,456)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	7	0.58
(1,393)	1:22:A:PRO:HA	1:22:A:PRO:HD2	6	0.58
(1,354)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	1	0.58
(1,354)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	9	0.58
(1,354)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.58
(1,248)	1:2:A:GLU:HA	1:2:A:GLU:HG2	10	0.58
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG2	5	0.58
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG3	5	0.58
(1,224)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	3	0.58
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	8	0.58
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	8	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	0.58
(1,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	2	0.58
(1,119)	1:8:A:TYR:HB3	1:9:A:ILE:H	2	0.58
(1,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	4	0.58
(1,119)	1:8:A:TYR:HB3	1:9:A:ILE:H	4	0.58
(1,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	5	0.58
(1,119)	1:8:A:TYR:HB3	1:9:A:ILE:H	5	0.58
(1,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.58
(1,119)	1:8:A:TYR:HB3	1:9:A:ILE:H	10	0.58
(1,53)	1:18:A:SER:H	1:18:A:SER:HB2	1	0.58
(1,53)	1:18:A:SER:H	1:18:A:SER:HB2	9	0.58
(1,53)	1:18:A:SER:H	1:18:A:SER:HB2	10	0.58
(4,38)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	7	0.57
(4,38)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	9	0.57
(3,33)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	4	0.57
(2,620)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	7	0.57
(2,620)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	9	0.57
(2,37)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	4	0.57
(1,612)	1:9:A:ILE:HG21	1:12:A:LEU:HB2	7	0.57
(1,612)	1:9:A:ILE:HG22	1:12:A:LEU:HB2	7	0.57
(1,612)	1:9:A:ILE:HG23	1:12:A:LEU:HB2	7	0.57
(1,612)	1:9:A:ILE:HG21	1:12:A:LEU:HB2	10	0.57
(1,612)	1:9:A:ILE:HG22	1:12:A:LEU:HB2	10	0.57
(1,612)	1:9:A:ILE:HG23	1:12:A:LEU:HB2	10	0.57
(1,590)	1:2:A:GLU:HG3	1:5:A:VAL:HG21	7	0.57
(1,590)	1:2:A:GLU:HG3	1:5:A:VAL:HG22	7	0.57
(1,590)	1:2:A:GLU:HG3	1:5:A:VAL:HG23	7	0.57
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB2	1	0.57
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB3	1	0.57
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB2	4	0.57
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB3	4	0.57
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG2	3	0.57
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG3	3	0.57
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG2	7	0.57
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG3	7	0.57
(1,313)	1:10:A:GLN:HA	1:10:A:GLN:HG3	10	0.57
(1,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	1	0.57
(1,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	3	0.57
(1,119)	1:8:A:TYR:HB3	1:9:A:ILE:H	3	0.57
(1,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	6	0.57
(1,119)	1:8:A:TYR:HB3	1:9:A:ILE:H	6	0.57
(1,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	7	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:8:A:TYR:HB3	1:9:A:ILE:H	7	0.57
(1,54)	1:18:A:SER:H	1:18:A:SER:HB3	8	0.57
(3,33)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	3	0.56
(2,37)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	3	0.56
(1,576)	1:10:A:GLN:HG2	1:11:A:TRP:HA	8	0.56
(1,571)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	4	0.56
(1,571)	1:24:A:PRO:HG3	1:25:A:CYS:HB2	4	0.56
(1,554)	1:4:A:CYS:HA	1:7:A:LEU:HG	10	0.56
(1,540)	1:2:A:GLU:HB2	1:6:A:ARG:H	5	0.56
(1,494)	1:22:A:PRO:HA	1:23:A:PRO:HD2	6	0.56
(1,494)	1:22:A:PRO:HA	1:23:A:PRO:HD2	7	0.56
(1,483)	1:7:A:LEU:HA	1:10:A:GLN:HB3	8	0.56
(1,443)	1:24:A:PRO:HA	1:24:A:PRO:HD3	6	0.56
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG2	6	0.56
(1,226)	1:8:A:TYR:H	1:24:A:PRO:HG3	6	0.56
(1,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	2	0.56
(1,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	0.56
(1,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	1	0.56
(1,119)	1:8:A:TYR:HB3	1:9:A:ILE:H	1	0.56
(1,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	8	0.56
(1,119)	1:8:A:TYR:HB3	1:9:A:ILE:H	8	0.56
(1,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	9	0.56
(1,119)	1:8:A:TYR:HB3	1:9:A:ILE:H	9	0.56
(4,38)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	4	0.55
(3,162)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	3	0.55
(2,620)	1:9:A:ILE:HG13	1:12:A:LEU:HB2	4	0.55
(2,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	3	0.55
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	6	0.55
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG3	6	0.55
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	6	0.55
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG3	6	0.55
(1,554)	1:4:A:CYS:HA	1:7:A:LEU:HG	2	0.55
(1,540)	1:2:A:GLU:HB2	1:6:A:ARG:H	3	0.55
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB2	9	0.55
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB3	9	0.55
(1,483)	1:7:A:LEU:HA	1:10:A:GLN:HB3	1	0.55
(1,482)	1:3:A:GLU:HA	1:6:A:ARG:HB3	8	0.55
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	7	0.55
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	7	0.55
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	7	0.55
(1,443)	1:24:A:PRO:HA	1:24:A:PRO:HD3	5	0.55
(1,415)	1:21:A:ARG:HA	1:22:A:PRO:HD3	1	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,415)	1:21:A:ARG:HA	1:22:A:PRO:HD3	5	0.55
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG2	8	0.55
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG3	8	0.55
(1,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	0.55
(3,141)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	4	0.54
(3,125)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	3	0.54
(2,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	4	0.54
(2,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	3	0.54
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	9	0.54
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	9	0.54
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	9	0.54
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	8	0.54
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	8	0.54
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	8	0.54
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	3	0.54
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG3	3	0.54
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	3	0.54
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG3	3	0.54
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	8	0.54
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG3	8	0.54
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	8	0.54
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG3	8	0.54
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB2	2	0.54
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB3	2	0.54
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB2	6	0.54
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB3	6	0.54
(1,393)	1:22:A:PRO:HA	1:22:A:PRO:HD2	1	0.54
(1,393)	1:22:A:PRO:HA	1:22:A:PRO:HD2	2	0.54
(1,393)	1:22:A:PRO:HA	1:22:A:PRO:HD2	5	0.54
(1,393)	1:22:A:PRO:HA	1:22:A:PRO:HD2	9	0.54
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG2	1	0.54
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG3	1	0.54
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG2	2	0.54
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG3	2	0.54
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG2	10	0.54
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG3	10	0.54
(1,278)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	6	0.54
(1,133)	1:11:A:TRP:HH2	1:23:A:PRO:HD2	1	0.54
(1,67)	1:3:A:GLU:H	1:3:A:GLU:HA	2	0.54
(1,67)	1:3:A:GLU:H	1:3:A:GLU:HA	9	0.54
(3,548)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	5	0.53
(2,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,612)	1:9:A:ILE:HG21	1:12:A:LEU:HB2	5	0.53
(1,612)	1:9:A:ILE:HG22	1:12:A:LEU:HB2	5	0.53
(1,612)	1:9:A:ILE:HG23	1:12:A:LEU:HB2	5	0.53
(1,571)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	6	0.53
(1,571)	1:24:A:PRO:HG3	1:25:A:CYS:HB2	6	0.53
(1,535)	1:9:A:ILE:HA	1:13:A:LYS:H	9	0.53
(1,529)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	3	0.53
(1,510)	1:12:A:LEU:HA	1:16:A:GLY:HA3	4	0.53
(1,483)	1:7:A:LEU:HA	1:10:A:GLN:HB3	3	0.53
(1,443)	1:24:A:PRO:HA	1:24:A:PRO:HD3	1	0.53
(1,415)	1:21:A:ARG:HA	1:22:A:PRO:HD3	2	0.53
(1,385)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	6	0.53
(1,352)	1:14:A:ASP:HA	1:14:A:ASP:HB2	6	0.53
(1,313)	1:10:A:GLN:HA	1:10:A:GLN:HG3	5	0.53
(1,274)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	10	0.53
(1,224)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	1	0.53
(1,217)	1:10:A:GLN:HG2	1:11:A:TRP:H	8	0.53
(1,149)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	3	0.53
(1,149)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	3	0.53
(1,53)	1:18:A:SER:H	1:18:A:SER:HB2	3	0.53
(3,564)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	8	0.52
(3,564)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	8	0.52
(3,564)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	8	0.52
(3,125)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	8	0.52
(2,598)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	8	0.52
(2,598)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	8	0.52
(2,598)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	8	0.52
(2,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	8	0.52
(1,612)	1:9:A:ILE:HG21	1:12:A:LEU:HB2	6	0.52
(1,612)	1:9:A:ILE:HG22	1:12:A:LEU:HB2	6	0.52
(1,612)	1:9:A:ILE:HG23	1:12:A:LEU:HB2	6	0.52
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	5	0.52
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	5	0.52
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	5	0.52
(1,518)	1:1:A:GLU:HA	1:1:A:GLU:HB2	5	0.52
(1,510)	1:12:A:LEU:HA	1:16:A:GLY:HA3	3	0.52
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB2	5	0.52
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB3	5	0.52
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	10	0.52
(1,389)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	10	0.52
(1,362)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	10	0.52
(1,199)	1:24:A:PRO:HD2	1:25:A:CYS:H	6	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	1	0.51
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	1	0.51
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	1	0.51
(3,125)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	1	0.51
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	1	0.51
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	1	0.51
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	1	0.51
(2,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	1	0.51
(1,612)	1:9:A:ILE:HG21	1:12:A:LEU:HB2	8	0.51
(1,612)	1:9:A:ILE:HG22	1:12:A:LEU:HB2	8	0.51
(1,612)	1:9:A:ILE:HG23	1:12:A:LEU:HB2	8	0.51
(1,575)	1:2:A:GLU:HB2	1:6:A:ARG:HA	6	0.51
(1,541)	1:2:A:GLU:HB3	1:6:A:ARG:H	10	0.51
(1,540)	1:2:A:GLU:HB2	1:6:A:ARG:H	8	0.51
(1,510)	1:12:A:LEU:HA	1:16:A:GLY:HA3	2	0.51
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB2	10	0.51
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB3	10	0.51
(1,483)	1:7:A:LEU:HA	1:10:A:GLN:HB3	2	0.51
(1,397)	1:22:A:PRO:HA	1:22:A:PRO:HG3	9	0.51
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	4	0.51
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	4	0.51
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	7	0.51
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	7	0.51
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	9	0.51
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	9	0.51
(1,352)	1:14:A:ASP:HA	1:14:A:ASP:HB2	7	0.51
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG2	4	0.51
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG3	4	0.51
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG2	5	0.51
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG3	5	0.51
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	5	0.51
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	5	0.51
(1,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.51
(1,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	9	0.51
(1,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	6	0.51
(1,60)	1:25:A:CYS:H	1:25:A:CYS:HB2	2	0.51
(1,36)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	1	0.51
(3,564)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	7	0.5
(3,564)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	7	0.5
(3,564)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	7	0.5
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	2	0.5
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	2	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	2	0.5
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.5
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.5
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.5
(3,141)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.5
(3,130)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	7	0.5
(3,130)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	7	0.5
(2,598)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	7	0.5
(2,598)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	7	0.5
(2,598)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	7	0.5
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	2	0.5
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	2	0.5
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	2	0.5
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	10	0.5
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	10	0.5
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	10	0.5
(2,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.5
(2,139)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	7	0.5
(2,139)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	7	0.5
(1,522)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	4	0.5
(1,510)	1:12:A:LEU:HA	1:16:A:GLY:HA3	6	0.5
(1,483)	1:7:A:LEU:HA	1:10:A:GLN:HB3	6	0.5
(1,415)	1:21:A:ARG:HA	1:22:A:PRO:HD3	9	0.5
(1,397)	1:22:A:PRO:HA	1:22:A:PRO:HG3	2	0.5
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	1	0.5
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	1	0.5
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	8	0.5
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	8	0.5
(1,352)	1:14:A:ASP:HA	1:14:A:ASP:HB2	3	0.5
(1,313)	1:10:A:GLN:HA	1:10:A:GLN:HG3	2	0.5
(1,278)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	5	0.5
(1,224)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	2	0.5
(1,207)	1:8:A:TYR:HD1	1:25:A:CYS:H	7	0.5
(1,207)	1:8:A:TYR:HD2	1:25:A:CYS:H	7	0.5
(1,199)	1:24:A:PRO:HD2	1:25:A:CYS:H	5	0.5
(1,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.5
(1,181)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	5	0.5
(1,36)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	7	0.5
(4,2)	1:6:A:ARG:H	1:6:A:ARG:HG2	9	0.49
(3,564)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	5	0.49
(3,564)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	5	0.49
(3,564)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,548)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	10	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	3	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	3	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	3	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	5	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	5	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	5	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	9	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	9	0.49
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	9	0.49
(3,141)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	3	0.49
(3,125)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.49
(2,598)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	5	0.49
(2,598)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	5	0.49
(2,598)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	5	0.49
(2,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	10	0.49
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	3	0.49
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	3	0.49
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	3	0.49
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	5	0.49
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	5	0.49
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	5	0.49
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	9	0.49
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	9	0.49
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	9	0.49
(2,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	3	0.49
(2,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.49
(2,15)	1:6:A:ARG:H	1:6:A:ARG:HG2	9	0.49
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	3	0.49
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	3	0.49
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	3	0.49
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	1	0.49
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG3	1	0.49
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	1	0.49
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG3	1	0.49
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD11	1	0.49
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD12	1	0.49
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD13	1	0.49
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD11	1	0.49
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD12	1	0.49
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD13	1	0.49
(1,529)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	9	0.49
(1,490)	1:14:A:ASP:HB3	1:19:A:SER:HB2	3	0.49
(1,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	6	0.49
(1,430)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	6	0.49
(1,397)	1:22:A:PRO:HA	1:22:A:PRO:HG3	5	0.49
(1,362)	1:17:A:PRO:HB2	1:17:A:PRO:HD2	9	0.49
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG2	9	0.49
(1,343)	1:13:A:LYS:HA	1:13:A:LYS:HG3	9	0.49
(1,312)	1:10:A:GLN:HA	1:10:A:GLN:HG2	10	0.49
(1,270)	1:6:A:ARG:HA	1:6:A:ARG:HG2	7	0.49
(1,224)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	9	0.49
(1,183)	1:11:A:TRP:HE3	1:12:A:LEU:HG	5	0.49
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	4	0.49
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	4	0.49
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	4	0.49
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	4	0.49
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	4	0.49
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	4	0.49
(1,149)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	8	0.49
(1,149)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	8	0.49
(1,123)	1:23:A:PRO:HB2	1:25:A:CYS:H	8	0.49
(1,113)	1:9:A:ILE:HA	1:12:A:LEU:H	9	0.49
(1,101)	1:24:A:PRO:HG2	1:25:A:CYS:H	10	0.49
(1,60)	1:25:A:CYS:H	1:25:A:CYS:HB2	3	0.49
(1,53)	1:18:A:SER:H	1:18:A:SER:HB2	6	0.49
(1,36)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	9	0.49
(1,1)	1:7:A:LEU:HB2	1:8:A:TYR:H	1	0.49
(1,1)	1:7:A:LEU:HB2	1:8:A:TYR:H	6	0.49
(3,548)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	1	0.48
(3,548)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	9	0.48
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	4	0.48
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	4	0.48
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	4	0.48
(3,130)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	6	0.48
(3,130)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	6	0.48
(2,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	1	0.48
(2,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	9	0.48
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	4	0.48
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	4	0.48
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	4	0.48
(2,139)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	6	0.48
(2,139)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,571)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	10	0.48
(1,571)	1:24:A:PRO:HG3	1:25:A:CYS:HB2	10	0.48
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	2	0.48
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG3	2	0.48
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	2	0.48
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG3	2	0.48
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD11	3	0.48
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD12	3	0.48
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD13	3	0.48
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD11	3	0.48
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD12	3	0.48
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD13	3	0.48
(1,521)	1:1:A:GLU:HA	1:1:A:GLU:HG3	2	0.48
(1,519)	1:1:A:GLU:HA	1:1:A:GLU:HB3	5	0.48
(1,501)	1:12:A:LEU:HA	1:16:A:GLY:HA2	2	0.48
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB2	7	0.48
(1,492)	1:5:A:VAL:HA	1:8:A:TYR:HB3	7	0.48
(1,481)	1:7:A:LEU:HA	1:10:A:GLN:HB2	4	0.48
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	10	0.48
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	10	0.48
(1,462)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	10	0.48
(1,443)	1:24:A:PRO:HA	1:24:A:PRO:HD3	2	0.48
(1,430)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	7	0.48
(1,384)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	10	0.48
(1,312)	1:10:A:GLN:HA	1:10:A:GLN:HG2	5	0.48
(1,286)	1:7:A:LEU:HA	1:7:A:LEU:HB3	4	0.48
(1,286)	1:7:A:LEU:HA	1:7:A:LEU:HB3	7	0.48
(1,278)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	3	0.48
(1,278)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.48
(1,271)	1:6:A:ARG:HA	1:6:A:ARG:HG3	1	0.48
(1,224)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	5	0.48
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	3	0.48
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	3	0.48
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	7	0.48
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	7	0.48
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	7	0.48
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	7	0.48
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	7	0.48
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	7	0.48
(1,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	9	0.48
(1,149)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	1	0.48
(1,149)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	1	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	2	0.48
(1,149)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	2	0.48
(1,149)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	5	0.48
(1,149)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	5	0.48
(1,149)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	10	0.48
(1,149)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	10	0.48
(1,60)	1:25:A:CYS:H	1:25:A:CYS:HB2	9	0.48
(3,564)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	10	0.47
(3,564)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	10	0.47
(3,564)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	10	0.47
(3,548)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	2	0.47
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	8	0.47
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	8	0.47
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	8	0.47
(3,463)	1:8:A:TYR:HA	1:11:A:TRP:HB2	4	0.47
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	4	0.47
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	5	0.47
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	7	0.47
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	9	0.47
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	10	0.47
(3,109)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	7	0.47
(2,598)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	10	0.47
(2,598)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	10	0.47
(2,598)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	10	0.47
(2,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	2	0.47
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	8	0.47
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	8	0.47
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	8	0.47
(2,493)	1:8:A:TYR:HA	1:11:A:TRP:HB2	4	0.47
(2,340)	1:12:A:LEU:HB3	1:13:A:LYS:H	4	0.47
(2,340)	1:12:A:LEU:HB3	1:13:A:LYS:H	5	0.47
(2,340)	1:12:A:LEU:HB3	1:13:A:LYS:H	7	0.47
(2,340)	1:12:A:LEU:HB3	1:13:A:LYS:H	9	0.47
(2,340)	1:12:A:LEU:HB3	1:13:A:LYS:H	10	0.47
(2,118)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	7	0.47
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	2	0.47
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	2	0.47
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	2	0.47
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	5	0.47
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG3	5	0.47
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	5	0.47
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG3	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	10	0.47
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG3	10	0.47
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	10	0.47
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG3	10	0.47
(1,547)	1:11:A:TRP:HH2	1:17:A:PRO:HB3	10	0.47
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD11	6	0.47
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD12	6	0.47
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD13	6	0.47
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD11	6	0.47
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD12	6	0.47
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD13	6	0.47
(1,522)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	2	0.47
(1,522)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	6	0.47
(1,519)	1:1:A:GLU:HA	1:1:A:GLU:HB3	3	0.47
(1,501)	1:12:A:LEU:HA	1:16:A:GLY:HA2	9	0.47
(1,484)	1:4:A:CYS:HA	1:7:A:LEU:HB3	1	0.47
(1,443)	1:24:A:PRO:HA	1:24:A:PRO:HD3	3	0.47
(1,443)	1:24:A:PRO:HA	1:24:A:PRO:HD3	9	0.47
(1,438)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	6	0.47
(1,372)	1:18:A:SER:HA	1:18:A:SER:HB2	1	0.47
(1,372)	1:18:A:SER:HA	1:18:A:SER:HB2	5	0.47
(1,372)	1:18:A:SER:HA	1:18:A:SER:HB2	9	0.47
(1,286)	1:7:A:LEU:HA	1:7:A:LEU:HB3	2	0.47
(1,286)	1:7:A:LEU:HA	1:7:A:LEU:HB3	10	0.47
(1,278)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	2	0.47
(1,278)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	8	0.47
(1,271)	1:6:A:ARG:HA	1:6:A:ARG:HG3	7	0.47
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG2	5	0.47
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	5	0.47
(1,123)	1:23:A:PRO:HB2	1:25:A:CYS:H	4	0.47
(1,60)	1:25:A:CYS:H	1:25:A:CYS:HB2	8	0.47
(1,38)	1:21:A:ARG:H	1:21:A:ARG:HB2	4	0.47
(1,38)	1:21:A:ARG:H	1:21:A:ARG:HB2	10	0.47
(1,36)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	4	0.47
(3,564)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	6	0.46
(3,564)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	6	0.46
(3,564)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	6	0.46
(3,548)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	8	0.46
(3,530)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	6	0.46
(3,478)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	4	0.46
(3,478)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	4	0.46
(3,478)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	2	0.46
(3,84)	1:10:A:GLN:HB2	1:11:A:TRP:H	4	0.46
(2,598)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	6	0.46
(2,598)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	6	0.46
(2,598)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	6	0.46
(2,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	8	0.46
(2,562)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	6	0.46
(2,508)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	4	0.46
(2,508)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	4	0.46
(2,508)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	4	0.46
(2,340)	1:12:A:LEU:HB3	1:13:A:LYS:H	2	0.46
(2,89)	1:10:A:GLN:HB2	1:11:A:TRP:H	4	0.46
(1,529)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	8	0.46
(1,438)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	7	0.46
(1,372)	1:18:A:SER:HA	1:18:A:SER:HB2	6	0.46
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	4	0.46
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	4	0.46
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	4	0.46
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD11	8	0.46
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD12	8	0.46
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD13	8	0.46
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	0.46
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	0.46
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	0.46
(1,270)	1:6:A:ARG:HA	1:6:A:ARG:HG2	1	0.46
(1,207)	1:8:A:TYR:HD1	1:25:A:CYS:H	10	0.46
(1,207)	1:8:A:TYR:HD2	1:25:A:CYS:H	10	0.46
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	2	0.46
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	2	0.46
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	2	0.46
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	2	0.46
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	2	0.46
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	2	0.46
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	9	0.46
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	9	0.46
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	9	0.46
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	9	0.46
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	9	0.46
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	9	0.46
(1,149)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	9	0.46
(1,149)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	9	0.46
(1,146)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:10:A:GLN:HB3	1:11:A:TRP:H	6	0.46
(1,53)	1:18:A:SER:H	1:18:A:SER:HB2	7	0.46
(4,22)	1:5:A:VAL:HG21	1:6:A:ARG:H	3	0.45
(4,22)	1:5:A:VAL:HG22	1:6:A:ARG:H	3	0.45
(4,22)	1:5:A:VAL:HG23	1:6:A:ARG:H	3	0.45
(3,564)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	4	0.45
(3,564)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	4	0.45
(3,564)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	4	0.45
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	7	0.45
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	7	0.45
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	7	0.45
(3,447)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	3	0.45
(3,427)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	6	0.45
(3,84)	1:10:A:GLN:HB2	1:11:A:TRP:H	2	0.45
(3,84)	1:10:A:GLN:HB2	1:11:A:TRP:H	3	0.45
(3,84)	1:10:A:GLN:HB2	1:11:A:TRP:H	7	0.45
(2,598)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	4	0.45
(2,598)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	4	0.45
(2,598)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	4	0.45
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	7	0.45
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	7	0.45
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	7	0.45
(2,477)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	3	0.45
(2,457)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	6	0.45
(2,232)	1:5:A:VAL:HG21	1:6:A:ARG:H	3	0.45
(2,232)	1:5:A:VAL:HG22	1:6:A:ARG:H	3	0.45
(2,232)	1:5:A:VAL:HG23	1:6:A:ARG:H	3	0.45
(2,89)	1:10:A:GLN:HB2	1:11:A:TRP:H	2	0.45
(2,89)	1:10:A:GLN:HB2	1:11:A:TRP:H	3	0.45
(2,89)	1:10:A:GLN:HB2	1:11:A:TRP:H	7	0.45
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	1	0.45
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	1	0.45
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	1	0.45
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	1	0.45
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	1	0.45
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	1	0.45
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	2	0.45
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	2	0.45
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	2	0.45
(1,580)	1:11:A:TRP:HB2	1:21:A:ARG:HD2	2	0.45
(1,547)	1:11:A:TRP:HH2	1:17:A:PRO:HB3	9	0.45
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD11	4	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD12	4	0.45
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD13	4	0.45
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD11	4	0.45
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD12	4	0.45
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD13	4	0.45
(1,529)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	4	0.45
(1,522)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	1	0.45
(1,510)	1:12:A:LEU:HA	1:16:A:GLY:HA3	8	0.45
(1,510)	1:12:A:LEU:HA	1:16:A:GLY:HA3	9	0.45
(1,443)	1:24:A:PRO:HA	1:24:A:PRO:HD3	4	0.45
(1,443)	1:24:A:PRO:HA	1:24:A:PRO:HD3	10	0.45
(1,406)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	1	0.45
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	5	0.45
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	5	0.45
(1,352)	1:14:A:ASP:HA	1:14:A:ASP:HB2	9	0.45
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	3	0.45
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	3	0.45
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	3	0.45
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	6	0.45
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	6	0.45
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	6	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	3	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	3	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	3	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	7	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	7	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	7	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	7	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	7	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	7	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	8	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	8	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	8	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	9	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	9	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	9	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	9	0.45
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	9	0.45
(1,278)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	7	0.45
(1,247)	1:2:A:GLU:HA	1:2:A:GLU:HB3	3	0.45
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	1	0.45
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	1	0.45
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG2	2	0.45
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	2	0.45
(1,174)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	6	0.45
(1,174)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	6	0.45
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	5	0.45
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	5	0.45
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	5	0.45
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	5	0.45
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	5	0.45
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	5	0.45
(1,149)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	4	0.45
(1,149)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	4	0.45
(1,149)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	7	0.45
(1,149)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	7	0.45
(1,146)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	1	0.45
(1,146)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	2	0.45
(1,146)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	4	0.45
(1,146)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	7	0.45
(1,146)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	8	0.45
(1,146)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	0.45
(1,1)	1:7:A:LEU:HB2	1:8:A:TYR:H	2	0.45
(1,1)	1:7:A:LEU:HB2	1:8:A:TYR:H	3	0.45
(1,1)	1:7:A:LEU:HB2	1:8:A:TYR:H	5	0.45
(1,1)	1:7:A:LEU:HB2	1:8:A:TYR:H	10	0.45
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	8	0.44
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	8	0.44
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	8	0.44
(4,22)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	0.44
(4,22)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	0.44
(4,22)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	0.44
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	6	0.44
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	6	0.44
(3,473)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	6	0.44
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	8	0.44
(3,84)	1:10:A:GLN:HB2	1:11:A:TRP:H	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	8	0.44
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	8	0.44
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	8	0.44
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD21	6	0.44
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD22	6	0.44
(2,503)	1:8:A:TYR:HB2	1:12:A:LEU:HD23	6	0.44
(2,340)	1:12:A:LEU:HB3	1:13:A:LYS:H	8	0.44
(2,232)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	0.44
(2,232)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	0.44
(2,232)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	0.44
(2,89)	1:10:A:GLN:HB2	1:11:A:TRP:H	8	0.44
(1,575)	1:2:A:GLU:HB2	1:6:A:ARG:HA	1	0.44
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	7	0.44
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG3	7	0.44
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	7	0.44
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG3	7	0.44
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	9	0.44
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG3	9	0.44
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	9	0.44
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG3	9	0.44
(1,510)	1:12:A:LEU:HA	1:16:A:GLY:HA3	5	0.44
(1,471)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	8	0.44
(1,443)	1:24:A:PRO:HA	1:24:A:PRO:HD3	7	0.44
(1,443)	1:24:A:PRO:HA	1:24:A:PRO:HD3	8	0.44
(1,438)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	4	0.44
(1,438)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	5	0.44
(1,438)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	8	0.44
(1,406)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	2	0.44
(1,406)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	9	0.44
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	6	0.44
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	6	0.44
(1,385)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	9	0.44
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	1	0.44
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	1	0.44
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	1	0.44
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	2	0.44
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	2	0.44
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	2	0.44
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	7	0.44
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	7	0.44
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	7	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	1	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	1	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	1	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	2	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	2	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	2	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	2	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	2	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	2	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	4	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	4	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	4	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	5	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	5	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	5	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	6	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	6	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	6	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	10	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	10	0.44
(1,290)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	10	0.44
(1,286)	1:7:A:LEU:HA	1:7:A:LEU:HB3	1	0.44
(1,286)	1:7:A:LEU:HA	1:7:A:LEU:HB3	3	0.44
(1,286)	1:7:A:LEU:HA	1:7:A:LEU:HB3	5	0.44
(1,286)	1:7:A:LEU:HA	1:7:A:LEU:HB3	9	0.44
(1,278)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	4	0.44
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	1	0.44
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	1	0.44
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	1	0.44
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	1	0.44
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	1	0.44
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	10	0.44
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	10	0.44
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	10	0.44
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	10	0.44
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	10	0.44
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	10	0.44
(1,149)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	6	0.44
(1,149)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	6	0.44
(1,146)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	3	0.44
(1,146)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	5	0.44
(1,146)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	9	0.44
(1,101)	1:24:A:PRO:HG2	1:25:A:CYS:H	7	0.44
(1,94)	1:9:A:ILE:H	1:9:A:ILE:HG13	4	0.44
(1,90)	1:10:A:GLN:HB3	1:11:A:TRP:H	8	0.44
(1,1)	1:7:A:LEU:HB2	1:8:A:TYR:H	7	0.44
(4,22)	1:5:A:VAL:HG21	1:6:A:ARG:H	7	0.43
(4,22)	1:5:A:VAL:HG22	1:6:A:ARG:H	7	0.43
(4,22)	1:5:A:VAL:HG23	1:6:A:ARG:H	7	0.43
(3,564)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	9	0.43
(3,564)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	9	0.43
(3,564)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	9	0.43
(3,463)	1:8:A:TYR:HA	1:11:A:TRP:HB2	7	0.43
(3,84)	1:10:A:GLN:HB2	1:11:A:TRP:H	9	0.43
(2,598)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	9	0.43
(2,598)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	9	0.43
(2,598)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	9	0.43
(2,493)	1:8:A:TYR:HA	1:11:A:TRP:HB2	7	0.43
(2,232)	1:5:A:VAL:HG21	1:6:A:ARG:H	7	0.43
(2,232)	1:5:A:VAL:HG22	1:6:A:ARG:H	7	0.43
(2,232)	1:5:A:VAL:HG23	1:6:A:ARG:H	7	0.43
(2,89)	1:10:A:GLN:HB2	1:11:A:TRP:H	9	0.43
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	4	0.43
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	4	0.43
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	4	0.43
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD11	9	0.43
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD12	9	0.43
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD13	9	0.43
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD11	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD12	9	0.43
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD13	9	0.43
(1,528)	1:16:A:GLY:H	1:19:A:SER:HB3	6	0.43
(1,522)	1:1:A:GLU:HB2	1:1:A:GLU:HG2	7	0.43
(1,438)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	2	0.43
(1,429)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	1	0.43
(1,406)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	5	0.43
(1,404)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	1	0.43
(1,404)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	9	0.43
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	2	0.43
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	2	0.43
(1,385)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	1	0.43
(1,385)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	4	0.43
(1,371)	1:18:A:SER:HA	1:18:A:SER:HB3	7	0.43
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	1	0.43
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	1	0.43
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	4	0.43
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	4	0.43
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	0.43
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	0.43
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	5	0.43
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	5	0.43
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	5	0.43
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	9	0.43
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	9	0.43
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	9	0.43
(1,313)	1:10:A:GLN:HA	1:10:A:GLN:HG3	6	0.43
(1,313)	1:10:A:GLN:HA	1:10:A:GLN:HG3	8	0.43
(1,286)	1:7:A:LEU:HA	1:7:A:LEU:HB3	6	0.43
(1,259)	1:4:A:CYS:HA	1:4:A:CYS:HB2	5	0.43
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	2	0.43
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	2	0.43
(1,181)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	9	0.43
(1,174)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	8	0.43
(1,174)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	8	0.43
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	8	0.43
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	8	0.43
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	8	0.43
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	8	0.43
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	8	0.43
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	8	0.43
(1,123)	1:23:A:PRO:HB2	1:25:A:CYS:H	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:9:A:ILE:HA	1:12:A:LEU:H	1	0.43
(1,94)	1:9:A:ILE:H	1:9:A:ILE:HG13	3	0.43
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	10	0.42
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	10	0.42
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	10	0.42
(4,23)	1:9:A:ILE:HD11	1:10:A:GLN:H	2	0.42
(4,23)	1:9:A:ILE:HD12	1:10:A:GLN:H	2	0.42
(4,23)	1:9:A:ILE:HD13	1:10:A:GLN:H	2	0.42
(3,564)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	2	0.42
(3,564)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	2	0.42
(3,564)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	2	0.42
(3,564)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	3	0.42
(3,564)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	3	0.42
(3,564)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	3	0.42
(3,447)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	4	0.42
(3,447)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	8	0.42
(3,427)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	3	0.42
(3,84)	1:10:A:GLN:HB2	1:11:A:TRP:H	1	0.42
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	10	0.42
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	10	0.42
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	10	0.42
(2,598)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	2	0.42
(2,598)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	2	0.42
(2,598)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	2	0.42
(2,598)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	3	0.42
(2,598)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	3	0.42
(2,598)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	3	0.42
(2,477)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	4	0.42
(2,477)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	8	0.42
(2,457)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	3	0.42
(2,233)	1:9:A:ILE:HD11	1:10:A:GLN:H	2	0.42
(2,233)	1:9:A:ILE:HD12	1:10:A:GLN:H	2	0.42
(2,233)	1:9:A:ILE:HD13	1:10:A:GLN:H	2	0.42
(2,89)	1:10:A:GLN:HB2	1:11:A:TRP:H	1	0.42
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	7	0.42
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	7	0.42
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	7	0.42
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	7	0.42
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	7	0.42
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	7	0.42
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD11	8	0.42
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD12	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD13	8	0.42
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD11	8	0.42
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD12	8	0.42
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD13	8	0.42
(1,501)	1:12:A:LEU:HA	1:16:A:GLY:HA2	7	0.42
(1,438)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	3	0.42
(1,438)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	9	0.42
(1,435)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	1	0.42
(1,435)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	10	0.42
(1,429)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.42
(1,406)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	3	0.42
(1,406)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	6	0.42
(1,406)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.42
(1,404)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	2	0.42
(1,404)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	5	0.42
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	3	0.42
(1,388)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	3	0.42
(1,372)	1:18:A:SER:HA	1:18:A:SER:HB2	8	0.42
(1,352)	1:14:A:ASP:HA	1:14:A:ASP:HB2	2	0.42
(1,352)	1:14:A:ASP:HA	1:14:A:ASP:HB2	4	0.42
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	5	0.42
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	5	0.42
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	9	0.42
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	9	0.42
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	8	0.42
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	8	0.42
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	8	0.42
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	10	0.42
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	10	0.42
(1,336)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	10	0.42
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	4	0.42
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	4	0.42
(1,181)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.42
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG2	9	0.42
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	9	0.42
(1,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	7	0.42
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	3	0.42
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	3	0.42
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	3	0.42
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	3	0.42
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	3	0.42
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:9:A:ILE:HA	1:12:A:LEU:H	4	0.42
(1,94)	1:9:A:ILE:H	1:9:A:ILE:HG13	1	0.42
(1,94)	1:9:A:ILE:H	1:9:A:ILE:HG13	6	0.42
(4,35)	1:5:A:VAL:HG21	1:9:A:ILE:HB	6	0.41
(4,35)	1:5:A:VAL:HG22	1:9:A:ILE:HB	6	0.41
(4,35)	1:5:A:VAL:HG23	1:9:A:ILE:HB	6	0.41
(4,23)	1:9:A:ILE:HD11	1:10:A:GLN:H	3	0.41
(4,23)	1:9:A:ILE:HD12	1:10:A:GLN:H	3	0.41
(4,23)	1:9:A:ILE:HD13	1:10:A:GLN:H	3	0.41
(3,427)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	7	0.41
(3,160)	1:23:A:PRO:HB3	1:25:A:CYS:H	4	0.41
(3,160)	1:23:A:PRO:HB3	1:25:A:CYS:H	9	0.41
(3,84)	1:10:A:GLN:HB2	1:11:A:TRP:H	6	0.41
(2,600)	1:5:A:VAL:HG21	1:9:A:ILE:HB	6	0.41
(2,600)	1:5:A:VAL:HG22	1:9:A:ILE:HB	6	0.41
(2,600)	1:5:A:VAL:HG23	1:9:A:ILE:HB	6	0.41
(2,457)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	7	0.41
(2,233)	1:9:A:ILE:HD11	1:10:A:GLN:H	3	0.41
(2,233)	1:9:A:ILE:HD12	1:10:A:GLN:H	3	0.41
(2,233)	1:9:A:ILE:HD13	1:10:A:GLN:H	3	0.41
(2,177)	1:23:A:PRO:HB3	1:25:A:CYS:H	4	0.41
(2,177)	1:23:A:PRO:HB3	1:25:A:CYS:H	9	0.41
(2,89)	1:10:A:GLN:HB2	1:11:A:TRP:H	6	0.41
(1,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	3	0.41
(1,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	7	0.41
(1,576)	1:10:A:GLN:HG2	1:11:A:TRP:HA	6	0.41
(1,568)	1:19:A:SER:HB3	1:21:A:ARG:HB3	5	0.41
(1,540)	1:2:A:GLU:HB2	1:6:A:ARG:H	1	0.41
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD11	2	0.41
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD12	2	0.41
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD13	2	0.41
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD11	2	0.41
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD12	2	0.41
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD13	2	0.41
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD11	7	0.41
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD12	7	0.41
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD13	7	0.41
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD11	7	0.41
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD12	7	0.41
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD13	7	0.41
(1,535)	1:9:A:ILE:HA	1:13:A:LYS:H	1	0.41
(1,529)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	6	0.41
(1,471)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	3	0.41
(1,471)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	4	0.41
(1,406)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	4	0.41
(1,406)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	8	0.41
(1,404)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.41
(1,352)	1:14:A:ASP:HA	1:14:A:ASP:HB2	5	0.41
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	2	0.41
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	2	0.41
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	7	0.41
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	7	0.41
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	8	0.41
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	8	0.41
(1,269)	1:6:A:ARG:HA	1:6:A:ARG:HB2	9	0.41
(1,248)	1:2:A:GLU:HA	1:2:A:GLU:HG2	6	0.41
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG2	1	0.41
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	1	0.41
(1,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	6	0.41
(1,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	1	0.41
(1,113)	1:9:A:ILE:HA	1:12:A:LEU:H	7	0.41
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	5	0.4
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	5	0.4
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	5	0.4
(4,23)	1:9:A:ILE:HD11	1:10:A:GLN:H	5	0.4
(4,23)	1:9:A:ILE:HD12	1:10:A:GLN:H	5	0.4
(4,23)	1:9:A:ILE:HD13	1:10:A:GLN:H	5	0.4
(3,564)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	1	0.4
(3,564)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	1	0.4
(3,564)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	1	0.4
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	1	0.4
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	6	0.4
(3,109)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	6	0.4
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	5	0.4
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	5	0.4
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	5	0.4
(2,598)	1:9:A:ILE:HG21	1:12:A:LEU:HB3	1	0.4
(2,598)	1:9:A:ILE:HG22	1:12:A:LEU:HB3	1	0.4
(2,598)	1:9:A:ILE:HG23	1:12:A:LEU:HB3	1	0.4
(2,340)	1:12:A:LEU:HB3	1:13:A:LYS:H	1	0.4
(2,340)	1:12:A:LEU:HB3	1:13:A:LYS:H	6	0.4
(2,233)	1:9:A:ILE:HD11	1:10:A:GLN:H	5	0.4
(2,233)	1:9:A:ILE:HD12	1:10:A:GLN:H	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,233)	1:9:A:ILE:HD13	1:10:A:GLN:H	5	0.4
(2,118)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	6	0.4
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	3	0.4
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	3	0.4
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	3	0.4
(1,539)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	4	0.4
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD11	10	0.4
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD12	10	0.4
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD13	10	0.4
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD11	10	0.4
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD12	10	0.4
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD13	10	0.4
(1,525)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	3	0.4
(1,521)	1:1:A:GLU:HA	1:1:A:GLU:HG3	1	0.4
(1,510)	1:12:A:LEU:HA	1:16:A:GLY:HA3	10	0.4
(1,501)	1:12:A:LEU:HA	1:16:A:GLY:HA2	1	0.4
(1,501)	1:12:A:LEU:HA	1:16:A:GLY:HA2	5	0.4
(1,495)	1:22:A:PRO:HA	1:23:A:PRO:HD3	1	0.4
(1,471)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	7	0.4
(1,456)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	1	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	1	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	1	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	2	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	2	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	3	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	3	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	4	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	4	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	5	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	5	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	6	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	6	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	7	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	7	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	8	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	8	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	9	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	9	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.4
(1,450)	1:24:A:PRO:HD2	1:24:A:PRO:HG3	10	0.4
(1,430)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	4	0.4
(1,430)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	8	0.4
(1,420)	1:23:A:PRO:HA	1:23:A:PRO:HD3	9	0.4
(1,404)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	3	0.4
(1,385)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	7	0.4
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	3	0.4
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	3	0.4
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	6	0.4
(1,348)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	6	0.4
(1,315)	1:10:A:GLN:HA	1:10:A:GLN:HB2	8	0.4
(1,280)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	1	0.4
(1,174)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	3	0.4
(1,174)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	3	0.4
(1,90)	1:10:A:GLN:HB3	1:11:A:TRP:H	2	0.4
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	6	0.39
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	6	0.39
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	6	0.39
(4,23)	1:9:A:ILE:HD11	1:10:A:GLN:H	8	0.39
(4,23)	1:9:A:ILE:HD12	1:10:A:GLN:H	8	0.39
(4,23)	1:9:A:ILE:HD13	1:10:A:GLN:H	8	0.39
(4,23)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.39
(4,23)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.39
(4,23)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.39
(4,22)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.39
(4,22)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.39
(4,22)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.39
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	6	0.39
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	6	0.39
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	6	0.39
(2,233)	1:9:A:ILE:HD11	1:10:A:GLN:H	8	0.39
(2,233)	1:9:A:ILE:HD12	1:10:A:GLN:H	8	0.39
(2,233)	1:9:A:ILE:HD13	1:10:A:GLN:H	8	0.39
(2,233)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.39
(2,233)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.39
(2,233)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.39
(2,232)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.39
(2,232)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.39
(2,232)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.39
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	4	0.39
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	4	0.39
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	4	0.39
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	5	0.39
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	5	0.39
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG2	4	0.39
(1,564)	1:8:A:TYR:HB2	1:24:A:PRO:HG3	4	0.39
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG2	4	0.39
(1,564)	1:8:A:TYR:HB3	1:24:A:PRO:HG3	4	0.39
(1,535)	1:9:A:ILE:HA	1:13:A:LYS:H	3	0.39
(1,535)	1:9:A:ILE:HA	1:13:A:LYS:H	4	0.39
(1,529)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	5	0.39
(1,523)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	7	0.39
(1,521)	1:1:A:GLU:HA	1:1:A:GLU:HG3	6	0.39
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD11	6	0.39
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD12	6	0.39
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD13	6	0.39
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD21	6	0.39
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD22	6	0.39
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD23	6	0.39
(1,481)	1:7:A:LEU:HA	1:10:A:GLN:HB2	9	0.39
(1,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	7	0.39
(1,429)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	3	0.39
(1,406)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	7	0.39
(1,404)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	4	0.39
(1,386)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	3	0.39
(1,286)	1:7:A:LEU:HA	1:7:A:LEU:HB3	8	0.39
(1,278)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	9	0.39
(1,228)	1:12:A:LEU:H	1:12:A:LEU:HB2	6	0.39
(1,174)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	1	0.39
(1,174)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	1	0.39
(1,174)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	9	0.39
(1,174)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	9	0.39
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG21	6	0.39
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG22	6	0.39
(1,168)	1:8:A:TYR:HD1	1:9:A:ILE:HG23	6	0.39
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG21	6	0.39
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG22	6	0.39
(1,168)	1:8:A:TYR:HD2	1:9:A:ILE:HG23	6	0.39
(1,123)	1:23:A:PRO:HB2	1:25:A:CYS:H	10	0.39
(1,113)	1:9:A:ILE:HA	1:12:A:LEU:H	2	0.39
(1,94)	1:9:A:ILE:H	1:9:A:ILE:HG13	8	0.39
(1,94)	1:9:A:ILE:H	1:9:A:ILE:HG13	9	0.39
(1,1)	1:7:A:LEU:HB2	1:8:A:TYR:H	4	0.39
(1,1)	1:7:A:LEU:HB2	1:8:A:TYR:H	9	0.39
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	9	0.38
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	9	0.38
(4,35)	1:5:A:VAL:HG21	1:9:A:ILE:HB	5	0.38
(4,35)	1:5:A:VAL:HG22	1:9:A:ILE:HB	5	0.38
(4,35)	1:5:A:VAL:HG23	1:9:A:ILE:HB	5	0.38
(4,35)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	0.38
(4,35)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	0.38
(4,35)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	0.38
(4,23)	1:9:A:ILE:HD11	1:10:A:GLN:H	9	0.38
(4,23)	1:9:A:ILE:HD12	1:10:A:GLN:H	9	0.38
(4,23)	1:9:A:ILE:HD13	1:10:A:GLN:H	9	0.38
(3,463)	1:8:A:TYR:HA	1:11:A:TRP:HB2	1	0.38
(3,463)	1:8:A:TYR:HA	1:11:A:TRP:HB2	2	0.38
(3,463)	1:8:A:TYR:HA	1:11:A:TRP:HB2	6	0.38
(3,312)	1:12:A:LEU:HB3	1:13:A:LYS:H	3	0.38
(3,177)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	6	0.38
(3,91)	1:7:A:LEU:H	1:10:A:GLN:HB2	8	0.38
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	9	0.38
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	9	0.38
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	9	0.38
(2,600)	1:5:A:VAL:HG21	1:9:A:ILE:HB	5	0.38
(2,600)	1:5:A:VAL:HG22	1:9:A:ILE:HB	5	0.38
(2,600)	1:5:A:VAL:HG23	1:9:A:ILE:HB	5	0.38
(2,600)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	0.38
(2,600)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	0.38
(2,600)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	0.38
(2,493)	1:8:A:TYR:HA	1:11:A:TRP:HB2	1	0.38
(2,493)	1:8:A:TYR:HA	1:11:A:TRP:HB2	2	0.38
(2,493)	1:8:A:TYR:HA	1:11:A:TRP:HB2	6	0.38
(2,340)	1:12:A:LEU:HB3	1:13:A:LYS:H	3	0.38
(2,233)	1:9:A:ILE:HD11	1:10:A:GLN:H	9	0.38
(2,233)	1:9:A:ILE:HD12	1:10:A:GLN:H	9	0.38
(2,233)	1:9:A:ILE:HD13	1:10:A:GLN:H	9	0.38
(2,197)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	6	0.38
(2,98)	1:7:A:LEU:H	1:10:A:GLN:HB2	8	0.38
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	9	0.38
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	9	0.38
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	9	0.38
(1,540)	1:2:A:GLU:HB2	1:6:A:ARG:H	7	0.38
(1,539)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	2	0.38
(1,526)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	1	0.38
(1,526)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,526)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	4	0.38
(1,526)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	5	0.38
(1,526)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	6	0.38
(1,526)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	7	0.38
(1,526)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	8	0.38
(1,526)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	9	0.38
(1,526)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	10	0.38
(1,523)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	1	0.38
(1,471)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	9	0.38
(1,456)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	3	0.38
(1,430)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	2	0.38
(1,429)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	2	0.38
(1,429)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	4	0.38
(1,429)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	5	0.38
(1,429)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	9	0.38
(1,404)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	6	0.38
(1,404)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	8	0.38
(1,371)	1:18:A:SER:HA	1:18:A:SER:HB3	10	0.38
(1,352)	1:14:A:ASP:HA	1:14:A:ASP:HB2	1	0.38
(1,352)	1:14:A:ASP:HA	1:14:A:ASP:HB2	8	0.38
(1,315)	1:10:A:GLN:HA	1:10:A:GLN:HB2	2	0.38
(1,214)	1:15:A:GLY:H	1:16:A:GLY:H	1	0.38
(1,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	5	0.38
(1,174)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	10	0.38
(1,174)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	10	0.38
(1,123)	1:23:A:PRO:HB2	1:25:A:CYS:H	9	0.38
(1,113)	1:9:A:ILE:HA	1:12:A:LEU:H	3	0.38
(1,94)	1:9:A:ILE:H	1:9:A:ILE:HG13	10	0.38
(1,90)	1:10:A:GLN:HB3	1:11:A:TRP:H	3	0.38
(1,1)	1:7:A:LEU:HB2	1:8:A:TYR:H	8	0.38
(4,35)	1:5:A:VAL:HG21	1:9:A:ILE:HB	3	0.37
(4,35)	1:5:A:VAL:HG22	1:9:A:ILE:HB	3	0.37
(4,35)	1:5:A:VAL:HG23	1:9:A:ILE:HB	3	0.37
(4,35)	1:5:A:VAL:HG21	1:9:A:ILE:HB	8	0.37
(4,35)	1:5:A:VAL:HG22	1:9:A:ILE:HB	8	0.37
(4,35)	1:5:A:VAL:HG23	1:9:A:ILE:HB	8	0.37
(4,35)	1:5:A:VAL:HG21	1:9:A:ILE:HB	9	0.37
(4,35)	1:5:A:VAL:HG22	1:9:A:ILE:HB	9	0.37
(4,35)	1:5:A:VAL:HG23	1:9:A:ILE:HB	9	0.37
(4,23)	1:9:A:ILE:HD11	1:10:A:GLN:H	1	0.37
(4,23)	1:9:A:ILE:HD12	1:10:A:GLN:H	1	0.37
(4,23)	1:9:A:ILE:HD13	1:10:A:GLN:H	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,22)	1:5:A:VAL:HG21	1:6:A:ARG:H	1	0.37
(4,22)	1:5:A:VAL:HG22	1:6:A:ARG:H	1	0.37
(4,22)	1:5:A:VAL:HG23	1:6:A:ARG:H	1	0.37
(4,22)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	0.37
(4,22)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	0.37
(4,22)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	0.37
(4,22)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	0.37
(4,22)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	0.37
(4,22)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	0.37
(4,22)	1:5:A:VAL:HG21	1:6:A:ARG:H	8	0.37
(4,22)	1:5:A:VAL:HG22	1:6:A:ARG:H	8	0.37
(4,22)	1:5:A:VAL:HG23	1:6:A:ARG:H	8	0.37
(3,485)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	0.37
(3,463)	1:8:A:TYR:HA	1:11:A:TRP:HB2	9	0.37
(3,447)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	10	0.37
(3,160)	1:23:A:PRO:HB3	1:25:A:CYS:H	8	0.37
(3,141)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	7	0.37
(3,130)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	2	0.37
(3,130)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	2	0.37
(2,600)	1:5:A:VAL:HG21	1:9:A:ILE:HB	3	0.37
(2,600)	1:5:A:VAL:HG22	1:9:A:ILE:HB	3	0.37
(2,600)	1:5:A:VAL:HG23	1:9:A:ILE:HB	3	0.37
(2,600)	1:5:A:VAL:HG21	1:9:A:ILE:HB	8	0.37
(2,600)	1:5:A:VAL:HG22	1:9:A:ILE:HB	8	0.37
(2,600)	1:5:A:VAL:HG23	1:9:A:ILE:HB	8	0.37
(2,600)	1:5:A:VAL:HG21	1:9:A:ILE:HB	9	0.37
(2,600)	1:5:A:VAL:HG22	1:9:A:ILE:HB	9	0.37
(2,600)	1:5:A:VAL:HG23	1:9:A:ILE:HB	9	0.37
(2,515)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	0.37
(2,493)	1:8:A:TYR:HA	1:11:A:TRP:HB2	9	0.37
(2,477)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	10	0.37
(2,233)	1:9:A:ILE:HD11	1:10:A:GLN:H	1	0.37
(2,233)	1:9:A:ILE:HD12	1:10:A:GLN:H	1	0.37
(2,233)	1:9:A:ILE:HD13	1:10:A:GLN:H	1	0.37
(2,232)	1:5:A:VAL:HG21	1:6:A:ARG:H	1	0.37
(2,232)	1:5:A:VAL:HG22	1:6:A:ARG:H	1	0.37
(2,232)	1:5:A:VAL:HG23	1:6:A:ARG:H	1	0.37
(2,232)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	0.37
(2,232)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	0.37
(2,232)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	0.37
(2,232)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	0.37
(2,232)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,232)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	0.37
(2,232)	1:5:A:VAL:HG21	1:6:A:ARG:H	8	0.37
(2,232)	1:5:A:VAL:HG22	1:6:A:ARG:H	8	0.37
(2,232)	1:5:A:VAL:HG23	1:6:A:ARG:H	8	0.37
(2,177)	1:23:A:PRO:HB3	1:25:A:CYS:H	8	0.37
(2,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	7	0.37
(2,139)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	2	0.37
(2,139)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	2	0.37
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	8	0.37
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	8	0.37
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	8	0.37
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD11	5	0.37
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD12	5	0.37
(1,538)	1:8:A:TYR:HD1	1:9:A:ILE:HD13	5	0.37
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD11	5	0.37
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD12	5	0.37
(1,538)	1:8:A:TYR:HD2	1:9:A:ILE:HD13	5	0.37
(1,526)	1:1:A:GLU:HB2	1:1:A:GLU:HB3	3	0.37
(1,495)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.37
(1,490)	1:14:A:ASP:HB3	1:19:A:SER:HB2	6	0.37
(1,471)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	5	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	4	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	4	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	6	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	6	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	7	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	7	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	8	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	8	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	9	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	9	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	10	0.37
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.37
(1,435)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	3	0.37
(1,435)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	9	0.37
(1,429)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	6	0.37
(1,429)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	8	0.37
(1,420)	1:23:A:PRO:HA	1:23:A:PRO:HD3	8	0.37
(1,409)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	1	0.37
(1,409)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	2	0.37
(1,409)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	3	0.37
(1,409)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	5	0.37
(1,409)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	6	0.37
(1,409)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	7	0.37
(1,409)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	8	0.37
(1,409)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	9	0.37
(1,409)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.37
(1,404)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	7	0.37
(1,386)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	2	0.37
(1,385)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	8	0.37
(1,371)	1:18:A:SER:HA	1:18:A:SER:HB3	2	0.37
(1,371)	1:18:A:SER:HA	1:18:A:SER:HB3	3	0.37
(1,369)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	9	0.37
(1,369)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.37
(1,332)	1:12:A:LEU:HB2	1:12:A:LEU:HG	4	0.37
(1,315)	1:10:A:GLN:HA	1:10:A:GLN:HB2	6	0.37
(1,280)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	9	0.37
(1,181)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	6	0.37
(1,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	9	0.37
(1,174)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	5	0.37
(1,174)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	5	0.37
(1,125)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	10	0.37
(1,94)	1:9:A:ILE:H	1:9:A:ILE:HG13	2	0.37
(1,94)	1:9:A:ILE:H	1:9:A:ILE:HG13	5	0.37
(1,94)	1:9:A:ILE:H	1:9:A:ILE:HG13	7	0.37
(1,38)	1:21:A:ARG:H	1:21:A:ARG:HB2	3	0.37
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	7	0.36
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	7	0.36
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	7	0.36
(4,35)	1:5:A:VAL:HG21	1:9:A:ILE:HB	1	0.36
(4,35)	1:5:A:VAL:HG22	1:9:A:ILE:HB	1	0.36
(4,35)	1:5:A:VAL:HG23	1:9:A:ILE:HB	1	0.36
(4,35)	1:5:A:VAL:HG21	1:9:A:ILE:HB	2	0.36
(4,35)	1:5:A:VAL:HG22	1:9:A:ILE:HB	2	0.36
(4,35)	1:5:A:VAL:HG23	1:9:A:ILE:HB	2	0.36
(4,22)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.36
(4,22)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.36
(4,22)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.36
(3,463)	1:8:A:TYR:HA	1:11:A:TRP:HB2	3	0.36
(3,425)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	10	0.36
(3,130)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	1	0.36
(3,130)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	1	0.36
(3,110)	1:8:A:TYR:HB2	1:9:A:ILE:H	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,110)	1:8:A:TYR:HB2	1:9:A:ILE:H	3	0.36
(3,110)	1:8:A:TYR:HB2	1:9:A:ILE:H	4	0.36
(3,110)	1:8:A:TYR:HB2	1:9:A:ILE:H	7	0.36
(3,110)	1:8:A:TYR:HB2	1:9:A:ILE:H	8	0.36
(3,110)	1:8:A:TYR:HB2	1:9:A:ILE:H	9	0.36
(3,31)	1:4:A:CYS:HB2	1:5:A:VAL:H	6	0.36
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	7	0.36
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	7	0.36
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	7	0.36
(2,600)	1:5:A:VAL:HG21	1:9:A:ILE:HB	1	0.36
(2,600)	1:5:A:VAL:HG22	1:9:A:ILE:HB	1	0.36
(2,600)	1:5:A:VAL:HG23	1:9:A:ILE:HB	1	0.36
(2,600)	1:5:A:VAL:HG21	1:9:A:ILE:HB	2	0.36
(2,600)	1:5:A:VAL:HG22	1:9:A:ILE:HB	2	0.36
(2,600)	1:5:A:VAL:HG23	1:9:A:ILE:HB	2	0.36
(2,493)	1:8:A:TYR:HA	1:11:A:TRP:HB2	3	0.36
(2,455)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	10	0.36
(2,232)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.36
(2,232)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.36
(2,232)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.36
(2,139)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	1	0.36
(2,139)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	1	0.36
(2,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	1	0.36
(2,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	3	0.36
(2,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	4	0.36
(2,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	7	0.36
(2,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	8	0.36
(2,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	9	0.36
(2,35)	1:4:A:CYS:HB2	1:5:A:VAL:H	6	0.36
(1,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	6	0.36
(1,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	6	0.36
(1,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	6	0.36
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	6	0.36
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	6	0.36
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	6	0.36
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	10	0.36
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	10	0.36
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	10	0.36
(1,535)	1:9:A:ILE:HA	1:13:A:LYS:H	8	0.36
(1,523)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	2	0.36
(1,523)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	6	0.36
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	1	0.36
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	2	0.36
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	2	0.36
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	3	0.36
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	3	0.36
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	5	0.36
(1,451)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	5	0.36
(1,439)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	1	0.36
(1,439)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.36
(1,435)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	2	0.36
(1,435)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	4	0.36
(1,435)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	5	0.36
(1,435)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	8	0.36
(1,429)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	7	0.36
(1,420)	1:23:A:PRO:HA	1:23:A:PRO:HD3	2	0.36
(1,377)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	1	0.36
(1,377)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	2	0.36
(1,377)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	3	0.36
(1,377)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	4	0.36
(1,377)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	5	0.36
(1,377)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	6	0.36
(1,377)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	7	0.36
(1,377)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	8	0.36
(1,377)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	9	0.36
(1,377)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	10	0.36
(1,371)	1:18:A:SER:HA	1:18:A:SER:HB3	4	0.36
(1,369)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	1	0.36
(1,369)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	2	0.36
(1,369)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	3	0.36
(1,369)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	4	0.36
(1,369)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	5	0.36
(1,369)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	6	0.36
(1,369)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	7	0.36
(1,369)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	8	0.36
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	9	0.36
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	9	0.36
(1,352)	1:14:A:ASP:HA	1:14:A:ASP:HB2	10	0.36
(1,332)	1:12:A:LEU:HB2	1:12:A:LEU:HG	1	0.36
(1,332)	1:12:A:LEU:HB2	1:12:A:LEU:HG	2	0.36
(1,332)	1:12:A:LEU:HB2	1:12:A:LEU:HG	3	0.36
(1,332)	1:12:A:LEU:HB2	1:12:A:LEU:HG	5	0.36
(1,332)	1:12:A:LEU:HB2	1:12:A:LEU:HG	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:10:A:GLN:HA	1:10:A:GLN:HB2	3	0.36
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.36
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.36
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.36
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.36
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.36
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.36
(1,207)	1:8:A:TYR:HD1	1:25:A:CYS:H	3	0.36
(1,207)	1:8:A:TYR:HD2	1:25:A:CYS:H	3	0.36
(1,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	9	0.36
(4,35)	1:5:A:VAL:HG21	1:9:A:ILE:HB	4	0.35
(4,35)	1:5:A:VAL:HG22	1:9:A:ILE:HB	4	0.35
(4,35)	1:5:A:VAL:HG23	1:9:A:ILE:HB	4	0.35
(4,35)	1:5:A:VAL:HG21	1:9:A:ILE:HB	7	0.35
(4,35)	1:5:A:VAL:HG22	1:9:A:ILE:HB	7	0.35
(4,35)	1:5:A:VAL:HG23	1:9:A:ILE:HB	7	0.35
(4,23)	1:9:A:ILE:HD11	1:10:A:GLN:H	6	0.35
(4,23)	1:9:A:ILE:HD12	1:10:A:GLN:H	6	0.35
(4,23)	1:9:A:ILE:HD13	1:10:A:GLN:H	6	0.35
(4,22)	1:5:A:VAL:HG21	1:6:A:ARG:H	9	0.35
(4,22)	1:5:A:VAL:HG22	1:6:A:ARG:H	9	0.35
(4,22)	1:5:A:VAL:HG23	1:6:A:ARG:H	9	0.35
(4,9)	1:12:A:LEU:H	1:13:A:LYS:HA	1	0.35
(3,485)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	0.35
(3,347)	1:19:A:SER:HA	1:19:A:SER:HB3	1	0.35
(3,347)	1:19:A:SER:HA	1:19:A:SER:HB3	4	0.35
(3,347)	1:19:A:SER:HA	1:19:A:SER:HB3	5	0.35
(3,347)	1:19:A:SER:HA	1:19:A:SER:HB3	8	0.35
(3,347)	1:19:A:SER:HA	1:19:A:SER:HB3	9	0.35
(3,347)	1:19:A:SER:HA	1:19:A:SER:HB3	10	0.35
(3,130)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	3	0.35
(3,130)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	3	0.35
(3,130)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	4	0.35
(3,130)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	4	0.35
(3,110)	1:8:A:TYR:HB2	1:9:A:ILE:H	2	0.35
(3,110)	1:8:A:TYR:HB2	1:9:A:ILE:H	5	0.35
(3,110)	1:8:A:TYR:HB2	1:9:A:ILE:H	6	0.35
(3,110)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.35
(2,600)	1:5:A:VAL:HG21	1:9:A:ILE:HB	4	0.35
(2,600)	1:5:A:VAL:HG22	1:9:A:ILE:HB	4	0.35
(2,600)	1:5:A:VAL:HG23	1:9:A:ILE:HB	4	0.35
(2,600)	1:5:A:VAL:HG21	1:9:A:ILE:HB	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,600)	1:5:A:VAL:HG22	1:9:A:ILE:HB	7	0.35
(2,600)	1:5:A:VAL:HG23	1:9:A:ILE:HB	7	0.35
(2,515)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	0.35
(2,375)	1:19:A:SER:HA	1:19:A:SER:HB3	1	0.35
(2,375)	1:19:A:SER:HA	1:19:A:SER:HB3	4	0.35
(2,375)	1:19:A:SER:HA	1:19:A:SER:HB3	5	0.35
(2,375)	1:19:A:SER:HA	1:19:A:SER:HB3	8	0.35
(2,375)	1:19:A:SER:HA	1:19:A:SER:HB3	9	0.35
(2,375)	1:19:A:SER:HA	1:19:A:SER:HB3	10	0.35
(2,233)	1:9:A:ILE:HD11	1:10:A:GLN:H	6	0.35
(2,233)	1:9:A:ILE:HD12	1:10:A:GLN:H	6	0.35
(2,233)	1:9:A:ILE:HD13	1:10:A:GLN:H	6	0.35
(2,232)	1:5:A:VAL:HG21	1:6:A:ARG:H	9	0.35
(2,232)	1:5:A:VAL:HG22	1:6:A:ARG:H	9	0.35
(2,232)	1:5:A:VAL:HG23	1:6:A:ARG:H	9	0.35
(2,139)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	3	0.35
(2,139)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	3	0.35
(2,139)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	4	0.35
(2,139)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	4	0.35
(2,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	2	0.35
(2,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	5	0.35
(2,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	6	0.35
(2,119)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.35
(2,114)	1:12:A:LEU:H	1:13:A:LYS:HA	1	0.35
(1,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.35
(1,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.35
(1,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.35
(1,568)	1:19:A:SER:HB3	1:21:A:ARG:HB3	1	0.35
(1,539)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	1	0.35
(1,525)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	5	0.35
(1,525)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	8	0.35
(1,523)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	10	0.35
(1,439)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	2	0.35
(1,439)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	3	0.35
(1,439)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	4	0.35
(1,439)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	5	0.35
(1,439)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	6	0.35
(1,439)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	7	0.35
(1,439)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	8	0.35
(1,439)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	9	0.35
(1,430)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	9	0.35
(1,420)	1:23:A:PRO:HA	1:23:A:PRO:HD3	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:23:A:PRO:HA	1:23:A:PRO:HD3	3	0.35
(1,420)	1:23:A:PRO:HA	1:23:A:PRO:HD3	5	0.35
(1,386)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	5	0.35
(1,380)	1:21:A:ARG:HA	1:21:A:ARG:HB2	7	0.35
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.35
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	10	0.35
(1,332)	1:12:A:LEU:HB2	1:12:A:LEU:HG	6	0.35
(1,332)	1:12:A:LEU:HB2	1:12:A:LEU:HG	7	0.35
(1,332)	1:12:A:LEU:HB2	1:12:A:LEU:HG	8	0.35
(1,332)	1:12:A:LEU:HB2	1:12:A:LEU:HG	10	0.35
(1,291)	1:7:A:LEU:HD11	1:7:A:LEU:HG	1	0.35
(1,291)	1:7:A:LEU:HD12	1:7:A:LEU:HG	1	0.35
(1,291)	1:7:A:LEU:HD13	1:7:A:LEU:HG	1	0.35
(1,291)	1:7:A:LEU:HD21	1:7:A:LEU:HG	1	0.35
(1,291)	1:7:A:LEU:HD22	1:7:A:LEU:HG	1	0.35
(1,291)	1:7:A:LEU:HD23	1:7:A:LEU:HG	1	0.35
(1,291)	1:7:A:LEU:HD11	1:7:A:LEU:HG	2	0.35
(1,291)	1:7:A:LEU:HD12	1:7:A:LEU:HG	2	0.35
(1,291)	1:7:A:LEU:HD13	1:7:A:LEU:HG	2	0.35
(1,291)	1:7:A:LEU:HD21	1:7:A:LEU:HG	2	0.35
(1,291)	1:7:A:LEU:HD22	1:7:A:LEU:HG	2	0.35
(1,291)	1:7:A:LEU:HD23	1:7:A:LEU:HG	2	0.35
(1,291)	1:7:A:LEU:HD11	1:7:A:LEU:HG	3	0.35
(1,291)	1:7:A:LEU:HD12	1:7:A:LEU:HG	3	0.35
(1,291)	1:7:A:LEU:HD13	1:7:A:LEU:HG	3	0.35
(1,291)	1:7:A:LEU:HD21	1:7:A:LEU:HG	3	0.35
(1,291)	1:7:A:LEU:HD22	1:7:A:LEU:HG	3	0.35
(1,291)	1:7:A:LEU:HD23	1:7:A:LEU:HG	3	0.35
(1,291)	1:7:A:LEU:HD11	1:7:A:LEU:HG	4	0.35
(1,291)	1:7:A:LEU:HD12	1:7:A:LEU:HG	4	0.35
(1,291)	1:7:A:LEU:HD13	1:7:A:LEU:HG	4	0.35
(1,291)	1:7:A:LEU:HD21	1:7:A:LEU:HG	4	0.35
(1,291)	1:7:A:LEU:HD22	1:7:A:LEU:HG	4	0.35
(1,291)	1:7:A:LEU:HD23	1:7:A:LEU:HG	4	0.35
(1,291)	1:7:A:LEU:HD11	1:7:A:LEU:HG	5	0.35
(1,291)	1:7:A:LEU:HD12	1:7:A:LEU:HG	5	0.35
(1,291)	1:7:A:LEU:HD13	1:7:A:LEU:HG	5	0.35
(1,291)	1:7:A:LEU:HD21	1:7:A:LEU:HG	5	0.35
(1,291)	1:7:A:LEU:HD22	1:7:A:LEU:HG	5	0.35
(1,291)	1:7:A:LEU:HD23	1:7:A:LEU:HG	5	0.35
(1,291)	1:7:A:LEU:HD11	1:7:A:LEU:HG	6	0.35
(1,291)	1:7:A:LEU:HD12	1:7:A:LEU:HG	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:7:A:LEU:HD13	1:7:A:LEU:HG	6	0.35
(1,291)	1:7:A:LEU:HD21	1:7:A:LEU:HG	6	0.35
(1,291)	1:7:A:LEU:HD22	1:7:A:LEU:HG	6	0.35
(1,291)	1:7:A:LEU:HD23	1:7:A:LEU:HG	6	0.35
(1,291)	1:7:A:LEU:HD11	1:7:A:LEU:HG	7	0.35
(1,291)	1:7:A:LEU:HD12	1:7:A:LEU:HG	7	0.35
(1,291)	1:7:A:LEU:HD13	1:7:A:LEU:HG	7	0.35
(1,291)	1:7:A:LEU:HD21	1:7:A:LEU:HG	7	0.35
(1,291)	1:7:A:LEU:HD22	1:7:A:LEU:HG	7	0.35
(1,291)	1:7:A:LEU:HD23	1:7:A:LEU:HG	7	0.35
(1,291)	1:7:A:LEU:HD11	1:7:A:LEU:HG	8	0.35
(1,291)	1:7:A:LEU:HD12	1:7:A:LEU:HG	8	0.35
(1,291)	1:7:A:LEU:HD13	1:7:A:LEU:HG	8	0.35
(1,291)	1:7:A:LEU:HD21	1:7:A:LEU:HG	8	0.35
(1,291)	1:7:A:LEU:HD22	1:7:A:LEU:HG	8	0.35
(1,291)	1:7:A:LEU:HD23	1:7:A:LEU:HG	8	0.35
(1,291)	1:7:A:LEU:HD11	1:7:A:LEU:HG	9	0.35
(1,291)	1:7:A:LEU:HD12	1:7:A:LEU:HG	9	0.35
(1,291)	1:7:A:LEU:HD13	1:7:A:LEU:HG	9	0.35
(1,291)	1:7:A:LEU:HD21	1:7:A:LEU:HG	9	0.35
(1,291)	1:7:A:LEU:HD22	1:7:A:LEU:HG	9	0.35
(1,291)	1:7:A:LEU:HD23	1:7:A:LEU:HG	9	0.35
(1,291)	1:7:A:LEU:HD11	1:7:A:LEU:HG	10	0.35
(1,291)	1:7:A:LEU:HD12	1:7:A:LEU:HG	10	0.35
(1,291)	1:7:A:LEU:HD13	1:7:A:LEU:HG	10	0.35
(1,291)	1:7:A:LEU:HD21	1:7:A:LEU:HG	10	0.35
(1,291)	1:7:A:LEU:HD22	1:7:A:LEU:HG	10	0.35
(1,291)	1:7:A:LEU:HD23	1:7:A:LEU:HG	10	0.35
(1,278)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	1	0.35
(1,271)	1:6:A:ARG:HA	1:6:A:ARG:HG3	10	0.35
(1,228)	1:12:A:LEU:H	1:12:A:LEU:HB2	7	0.35
(1,228)	1:12:A:LEU:H	1:12:A:LEU:HB2	8	0.35
(1,228)	1:12:A:LEU:H	1:12:A:LEU:HB2	10	0.35
(1,217)	1:10:A:GLN:HG2	1:11:A:TRP:H	2	0.35
(1,217)	1:10:A:GLN:HG2	1:11:A:TRP:H	6	0.35
(1,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	4	0.35
(1,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	7	0.35
(1,123)	1:23:A:PRO:HB2	1:25:A:CYS:H	6	0.35
(1,113)	1:9:A:ILE:HA	1:12:A:LEU:H	8	0.35
(1,113)	1:9:A:ILE:HA	1:12:A:LEU:H	10	0.35
(1,60)	1:25:A:CYS:H	1:25:A:CYS:HB2	6	0.35
(1,53)	1:18:A:SER:H	1:18:A:SER:HB2	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	3	0.34
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	3	0.34
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	3	0.34
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HB2	9	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
(3,485)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	0.34
(3,463)	1:8:A:TYR:HA	1:11:A:TRP:HB2	5	0.34
(3,427)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	10	0.34
(3,347)	1:19:A:SER:HA	1:19:A:SER:HB3	2	0.34
(3,339)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	1	0.34
(3,339)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	2	0.34
(3,339)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	3	0.34
(3,339)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	5	0.34
(3,339)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	6	0.34
(3,339)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	7	0.34
(3,339)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	8	0.34
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	3	0.34
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	3	0.34
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	3	0.34
(2,515)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	0.34
(2,493)	1:8:A:TYR:HA	1:11:A:TRP:HB2	5	0.34
(2,457)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	10	0.34
(2,375)	1:19:A:SER:HA	1:19:A:SER:HB3	2	0.34
(2,367)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	1	0.34
(2,367)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	2	0.34
(2,367)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	3	0.34
(2,367)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	5	0.34
(2,367)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	6	0.34
(2,367)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	7	0.34
(2,367)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	8	0.34
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	9	0.34
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.34
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.34
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.34
(1,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	0.34
(1,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	0.34
(1,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	0.34
(1,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	2	0.34
(1,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	2	0.34
(1,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG11	4	0.34
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG12	4	0.34
(1,599)	1:2:A:GLU:HB2	1:5:A:VAL:HG13	4	0.34
(1,558)	1:2:A:GLU:HA	1:5:A:VAL:HB	4	0.34
(1,541)	1:2:A:GLU:HB3	1:6:A:ARG:H	4	0.34
(1,539)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	9	0.34
(1,537)	1:5:A:VAL:HG11	1:9:A:ILE:H	1	0.34
(1,537)	1:5:A:VAL:HG12	1:9:A:ILE:H	1	0.34
(1,537)	1:5:A:VAL:HG13	1:9:A:ILE:H	1	0.34
(1,537)	1:5:A:VAL:HG11	1:9:A:ILE:H	6	0.34
(1,537)	1:5:A:VAL:HG12	1:9:A:ILE:H	6	0.34
(1,537)	1:5:A:VAL:HG13	1:9:A:ILE:H	6	0.34
(1,535)	1:9:A:ILE:HA	1:13:A:LYS:H	10	0.34
(1,525)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	9	0.34
(1,506)	1:18:A:SER:HB2	1:19:A:SER:H	10	0.34
(1,501)	1:12:A:LEU:HA	1:16:A:GLY:HA2	4	0.34
(1,471)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	1	0.34
(1,471)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	10	0.34
(1,463)	1:13:A:LYS:HA	1:13:A:LYS:HE2	4	0.34
(1,435)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	6	0.34
(1,435)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	7	0.34
(1,387)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	10	0.34
(1,380)	1:21:A:ARG:HA	1:21:A:ARG:HB2	1	0.34
(1,380)	1:21:A:ARG:HA	1:21:A:ARG:HB2	6	0.34
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.34
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.34
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.34
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.34
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.34
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.34
(1,247)	1:2:A:GLU:HA	1:2:A:GLU:HB3	6	0.34
(1,228)	1:12:A:LEU:H	1:12:A:LEU:HB2	3	0.34
(1,228)	1:12:A:LEU:H	1:12:A:LEU:HB2	5	0.34
(1,207)	1:8:A:TYR:HD1	1:25:A:CYS:H	2	0.34
(1,207)	1:8:A:TYR:HD2	1:25:A:CYS:H	2	0.34
(1,181)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	7	0.34
(1,174)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	2	0.34
(1,174)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	2	0.34
(1,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	5	0.34
(1,97)	1:12:A:LEU:H	1:12:A:LEU:HG	6	0.34
(1,97)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.34
(1,61)	1:25:A:CYS:H	1:25:A:CYS:HB3	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:21:A:ARG:H	1:21:A:ARG:HB2	8	0.34
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	8	0.34
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	8	0.34
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	8	0.34
(4,23)	1:9:A:ILE:HD11	1:10:A:GLN:H	7	0.33
(4,23)	1:9:A:ILE:HD12	1:10:A:GLN:H	7	0.33
(4,23)	1:9:A:ILE:HD13	1:10:A:GLN:H	7	0.33
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	10	0.33
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	10	0.33
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	10	0.33
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	10	0.33
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	10	0.33
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	10	0.33
(4,9)	1:12:A:LEU:H	1:13:A:LYS:HA	6	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	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	6	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.33
(4,1)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	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
(3,463)	1:8:A:TYR:HA	1:11:A:TRP:HB2	10	0.33
(3,339)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	4	0.33
(3,175)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	4	0.33
(2,493)	1:8:A:TYR:HA	1:11:A:TRP:HB2	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,367)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	4	0.33
(2,233)	1:9:A:ILE:HD11	1:10:A:GLN:H	7	0.33
(2,233)	1:9:A:ILE:HD12	1:10:A:GLN:H	7	0.33
(2,233)	1:9:A:ILE:HD13	1:10:A:GLN:H	7	0.33
(2,195)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	4	0.33
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	10	0.33
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	10	0.33
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	10	0.33
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	10	0.33
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	10	0.33
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	10	0.33
(2,114)	1:12:A:LEU:H	1:13:A:LYS:HA	6	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.33
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.33
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	10	0.33
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	10	0.33
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	10	0.33
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	2	0.33
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	2	0.33
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,576)	1:10:A:GLN:HG2	1:11:A:TRP:HA	2	0.33
(1,535)	1:9:A:ILE:HA	1:13:A:LYS:H	2	0.33
(1,523)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	5	0.33
(1,501)	1:12:A:LEU:HA	1:16:A:GLY:HA2	10	0.33
(1,481)	1:7:A:LEU:HA	1:10:A:GLN:HB2	10	0.33
(1,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	8	0.33
(1,420)	1:23:A:PRO:HA	1:23:A:PRO:HD3	4	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD11	5	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD12	5	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD13	5	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.33
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.33
(1,247)	1:2:A:GLU:HA	1:2:A:GLU:HB3	4	0.33
(1,243)	1:11:A:TRP:HB3	1:12:A:LEU:H	5	0.33
(1,228)	1:12:A:LEU:H	1:12:A:LEU:HB2	1	0.33
(1,207)	1:8:A:TYR:HD1	1:25:A:CYS:H	8	0.33
(1,207)	1:8:A:TYR:HD2	1:25:A:CYS:H	8	0.33
(1,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	7	0.33
(1,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	7	0.33
(1,38)	1:21:A:ARG:H	1:21:A:ARG:HB2	5	0.33
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	4	0.32
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	4	0.32
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	4	0.32
(4,23)	1:9:A:ILE:HD11	1:10:A:GLN:H	4	0.32
(4,23)	1:9:A:ILE:HD12	1:10:A:GLN:H	4	0.32
(4,23)	1:9:A:ILE:HD13	1:10:A:GLN:H	4	0.32
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	9	0.32
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	9	0.32
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	9	0.32
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	9	0.32
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	9	0.32
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	9	0.32
(4,9)	1:12:A:LEU:H	1:13:A:LYS:HA	3	0.32
(4,9)	1:12:A:LEU:H	1:13:A:LYS:HA	8	0.32
(4,2)	1:6:A:ARG:H	1:6:A:ARG:HG2	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(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
(3,175)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	3	0.32
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	4	0.32
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	4	0.32
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	4	0.32
(2,233)	1:9:A:ILE:HD11	1:10:A:GLN:H	4	0.32
(2,233)	1:9:A:ILE:HD12	1:10:A:GLN:H	4	0.32
(2,233)	1:9:A:ILE:HD13	1:10:A:GLN:H	4	0.32
(2,195)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	3	0.32
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	9	0.32
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	9	0.32
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	9	0.32
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	9	0.32
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	9	0.32
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	9	0.32
(2,114)	1:12:A:LEU:H	1:13:A:LYS:HA	3	0.32
(2,114)	1:12:A:LEU:H	1:13:A:LYS:HA	8	0.32
(2,15)	1:6:A:ARG:H	1:6:A:ARG:HG2	2	0.32
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.32
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.32
(2,4)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.32
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	8	0.32
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	8	0.32
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	8	0.32
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	7	0.32
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	7	0.32
(1,525)	1:1:A:GLU:HB3	1:1:A:GLU:HG2	10	0.32
(1,523)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	4	0.32
(1,523)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	8	0.32
(1,512)	1:23:A:PRO:HA	1:24:A:PRO:HD2	3	0.32
(1,501)	1:12:A:LEU:HA	1:16:A:GLY:HA2	3	0.32
(1,380)	1:21:A:ARG:HA	1:21:A:ARG:HB2	9	0.32
(1,269)	1:6:A:ARG:HA	1:6:A:ARG:HB2	10	0.32
(1,228)	1:12:A:LEU:H	1:12:A:LEU:HB2	2	0.32
(1,228)	1:12:A:LEU:H	1:12:A:LEU:HB2	4	0.32
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	6	0.32
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	6	0.32
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	7	0.32
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	7	0.32
(1,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	5	0.32
(1,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	6	0.32
(1,97)	1:12:A:LEU:H	1:12:A:LEU:HG	3	0.32
(1,97)	1:12:A:LEU:H	1:12:A:LEU:HG	7	0.32
(1,97)	1:12:A:LEU:H	1:12:A:LEU:HG	9	0.32
(1,97)	1:12:A:LEU:H	1:12:A:LEU:HG	10	0.32
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	5	0.31
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	5	0.31
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	5	0.31
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	5	0.31
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	5	0.31
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	5	0.31
(4,9)	1:12:A:LEU:H	1:13:A:LYS:HA	4	0.31
(4,2)	1:6:A:ARG:H	1:6:A:ARG:HG2	10	0.31
(3,202)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	9	0.31
(3,160)	1:23:A:PRO:HB3	1:25:A:CYS:H	3	0.31
(3,130)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	8	0.31
(3,130)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	8	0.31
(3,130)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	9	0.31
(3,130)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	9	0.31
(3,130)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	10	0.31
(3,130)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	10	0.31
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.31
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.31
(2,222)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	9	0.31
(2,177)	1:23:A:PRO:HB3	1:25:A:CYS:H	3	0.31
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	5	0.31
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	5	0.31
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	5	0.31
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	5	0.31
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	5	0.31
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	5	0.31
(2,139)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	8	0.31
(2,139)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	8	0.31
(2,139)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	9	0.31
(2,139)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	9	0.31
(2,139)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	10	0.31
(2,139)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	10	0.31
(2,114)	1:12:A:LEU:H	1:13:A:LYS:HA	4	0.31
(2,22)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.31
(2,22)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.31
(2,15)	1:6:A:ARG:H	1:6:A:ARG:HG2	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	5	0.31
(1,535)	1:9:A:ILE:HA	1:13:A:LYS:H	5	0.31
(1,512)	1:23:A:PRO:HA	1:24:A:PRO:HD2	5	0.31
(1,512)	1:23:A:PRO:HA	1:24:A:PRO:HD2	10	0.31
(1,510)	1:12:A:LEU:HA	1:16:A:GLY:HA3	7	0.31
(1,430)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	3	0.31
(1,324)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	1	0.31
(1,324)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	2	0.31
(1,324)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	3	0.31
(1,324)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	4	0.31
(1,324)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	5	0.31
(1,324)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	6	0.31
(1,324)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	7	0.31
(1,280)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	4	0.31
(1,280)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	7	0.31
(1,247)	1:2:A:GLU:HA	1:2:A:GLU:HB3	2	0.31
(1,247)	1:2:A:GLU:HA	1:2:A:GLU:HB3	5	0.31
(1,228)	1:12:A:LEU:H	1:12:A:LEU:HB2	9	0.31
(1,214)	1:15:A:GLY:H	1:16:A:GLY:H	3	0.31
(1,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	4	0.31
(1,174)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	7	0.31
(1,174)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	7	0.31
(1,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	2	0.31
(1,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	3	0.31
(1,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	8	0.31
(1,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	9	0.31
(1,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.31
(1,134)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	6	0.31
(1,113)	1:9:A:ILE:HA	1:12:A:LEU:H	5	0.31
(1,113)	1:9:A:ILE:HA	1:12:A:LEU:H	6	0.31
(1,90)	1:10:A:GLN:HB3	1:11:A:TRP:H	1	0.31
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	6	0.3
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	6	0.3
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	6	0.3
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	6	0.3
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	6	0.3
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	6	0.3
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	6	0.3
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	6	0.3
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	6	0.3
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	10	0.3
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	10	0.3
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	10	0.3
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	10	0.3
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	10	0.3
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	10	0.3
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	10	0.3
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	10	0.3
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	8	0.3
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	8	0.3
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	8	0.3
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	8	0.3
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	8	0.3
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	8	0.3
(4,9)	1:12:A:LEU:H	1:13:A:LYS:HA	2	0.3
(4,9)	1:12:A:LEU:H	1:13:A:LYS:HA	5	0.3
(4,9)	1:12:A:LEU:H	1:13:A:LYS:HA	7	0.3
(4,9)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.3
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	5	0.3
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	5	0.3
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	5	0.3
(3,202)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	4	0.3
(3,177)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	1	0.3
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	5	0.3
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	6	0.3
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	6	0.3
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	6	0.3
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	6	0.3
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	6	0.3
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	6	0.3
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	6	0.3
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	6	0.3
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	6	0.3
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	10	0.3
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	10	0.3
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	10	0.3
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	10	0.3
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	10	0.3
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	10	0.3
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	10	0.3
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	10	0.3
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	10	0.3
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	5	0.3
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	5	0.3
(2,222)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	4	0.3
(2,197)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	1	0.3
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	8	0.3
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	8	0.3
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	8	0.3
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	8	0.3
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	8	0.3
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	8	0.3
(2,114)	1:12:A:LEU:H	1:13:A:LYS:HA	2	0.3
(2,114)	1:12:A:LEU:H	1:13:A:LYS:HA	5	0.3
(2,114)	1:12:A:LEU:H	1:13:A:LYS:HA	7	0.3
(2,114)	1:12:A:LEU:H	1:13:A:LYS:HA	10	0.3
(2,22)	1:10:A:GLN:H	1:10:A:GLN:HG2	5	0.3
(1,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	9	0.3
(1,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	9	0.3
(1,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	9	0.3
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD11	3	0.3
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD12	3	0.3
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD13	3	0.3
(1,582)	1:1:A:GLU:HB3	1:2:A:GLU:HG3	6	0.3
(1,571)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	8	0.3
(1,571)	1:24:A:PRO:HG3	1:25:A:CYS:HB2	8	0.3
(1,568)	1:19:A:SER:HB3	1:21:A:ARG:HB3	2	0.3
(1,541)	1:2:A:GLU:HB3	1:6:A:ARG:H	6	0.3
(1,537)	1:5:A:VAL:HG11	1:9:A:ILE:H	8	0.3
(1,537)	1:5:A:VAL:HG12	1:9:A:ILE:H	8	0.3
(1,537)	1:5:A:VAL:HG13	1:9:A:ILE:H	8	0.3
(1,537)	1:5:A:VAL:HG11	1:9:A:ILE:H	9	0.3
(1,537)	1:5:A:VAL:HG12	1:9:A:ILE:H	9	0.3
(1,537)	1:5:A:VAL:HG13	1:9:A:ILE:H	9	0.3
(1,537)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	0.3
(1,537)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	0.3
(1,537)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	0.3
(1,535)	1:9:A:ILE:HA	1:13:A:LYS:H	7	0.3
(1,521)	1:1:A:GLU:HA	1:1:A:GLU:HG3	4	0.3
(1,512)	1:23:A:PRO:HA	1:24:A:PRO:HD2	2	0.3
(1,512)	1:23:A:PRO:HA	1:24:A:PRO:HD2	6	0.3
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	7	0.3
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	7	0.3
(1,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	10	0.3
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	9	0.3
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	9	0.3
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	10	0.3
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	10	0.3
(1,324)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	8	0.3
(1,324)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	9	0.3
(1,324)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.3
(1,304)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	2	0.3
(1,292)	1:7:A:LEU:HB2	1:7:A:LEU:HG	8	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD11	4	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD12	4	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD13	4	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD11	6	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD12	6	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD13	6	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.3
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.3
(1,207)	1:8:A:TYR:HD1	1:25:A:CYS:H	1	0.3
(1,207)	1:8:A:TYR:HD2	1:25:A:CYS:H	1	0.3
(1,181)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	1	0.3
(1,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	8	0.3
(1,150)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	1	0.3
(1,97)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.3
(1,97)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.3
(1,97)	1:12:A:LEU:H	1:12:A:LEU:HG	5	0.3
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	3	0.29
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	3	0.29
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	3	0.29
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	3	0.29
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	3	0.29
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	3	0.29
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	7	0.29
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	7	0.29
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	7	0.29
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	7	0.29
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	7	0.29
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,485)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	0.29
(3,485)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.29
(3,178)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	6	0.29
(3,178)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	7	0.29
(3,160)	1:23:A:PRO:HB3	1:25:A:CYS:H	2	0.29
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	4	0.29
(2,515)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	0.29
(2,515)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.29
(2,198)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	6	0.29
(2,198)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	7	0.29
(2,177)	1:23:A:PRO:HB3	1:25:A:CYS:H	2	0.29
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	3	0.29
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	3	0.29
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	3	0.29
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	3	0.29
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	3	0.29
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	3	0.29
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	7	0.29
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	7	0.29
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	7	0.29
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	7	0.29
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	7	0.29
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	7	0.29
(2,22)	1:10:A:GLN:H	1:10:A:GLN:HG2	4	0.29
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD11	8	0.29
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD12	8	0.29
(1,596)	1:2:A:GLU:HB3	1:9:A:ILE:HD13	8	0.29
(1,539)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	10	0.29
(1,521)	1:1:A:GLU:HA	1:1:A:GLU:HG3	7	0.29
(1,384)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	4	0.29
(1,380)	1:21:A:ARG:HA	1:21:A:ARG:HB2	2	0.29
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	4	0.29
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	4	0.29
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	6	0.29
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	6	0.29
(1,315)	1:10:A:GLN:HA	1:10:A:GLN:HB2	1	0.29
(1,315)	1:10:A:GLN:HA	1:10:A:GLN:HB2	9	0.29
(1,304)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	1	0.29
(1,304)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	3	0.29
(1,304)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	4	0.29
(1,304)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	5	0.29
(1,304)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,304)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	7	0.29
(1,304)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	8	0.29
(1,304)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	9	0.29
(1,304)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	10	0.29
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD11	7	0.29
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD12	7	0.29
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD13	7	0.29
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.29
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.29
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.29
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG2	1	0.29
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG3	1	0.29
(1,247)	1:2:A:GLU:HA	1:2:A:GLU:HB3	9	0.29
(1,243)	1:11:A:TRP:HB3	1:12:A:LEU:H	9	0.29
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	6	0.29
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	6	0.29
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	6	0.29
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	6	0.29
(1,157)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	7	0.29
(1,157)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	7	0.29
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD21	2	0.29
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD22	2	0.29
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD23	2	0.29
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	1	0.28
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	1	0.28
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	1	0.28
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	1	0.28
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	1	0.28
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	1	0.28
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	1	0.28
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	1	0.28
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	1	0.28
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	2	0.28
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	2	0.28
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	2	0.28
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	2	0.28
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	2	0.28
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	2	0.28
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	2	0.28
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	2	0.28
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	2	0.28
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	9	0.28
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	9	0.28
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	9	0.28
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	9	0.28
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	9	0.28
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	9	0.28
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	9	0.28
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	9	0.28
(4,20)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	5	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	5	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	5	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	5	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	8	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	8	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	8	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	9	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	9	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	9	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	10	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	10	0.28
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	10	0.28
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	1	0.28
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	1	0.28
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	1	0.28
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	1	0.28
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	1	0.28
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	1	0.28
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	4	0.28
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	4	0.28
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	4	0.28
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	4	0.28
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	4	0.28
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	4	0.28
(4,9)	1:12:A:LEU:H	1:13:A:LYS:HA	9	0.28
(4,8)	1:10:A:GLN:HA	1:11:A:TRP:H	5	0.28
(3,478)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	5	0.28
(3,478)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	5	0.28
(3,478)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	5	0.28
(3,427)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	5	0.28
(3,425)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	1	0.28
(3,202)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	5	0.28
(3,160)	1:23:A:PRO:HB3	1:25:A:CYS:H	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	1	0.28
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	1	0.28
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	1	0.28
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	1	0.28
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	1	0.28
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	1	0.28
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	1	0.28
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	1	0.28
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	1	0.28
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	2	0.28
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	2	0.28
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	2	0.28
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	2	0.28
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	2	0.28
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	2	0.28
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	2	0.28
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	2	0.28
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	2	0.28
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	9	0.28
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	9	0.28
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	9	0.28
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	9	0.28
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	9	0.28
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	9	0.28
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	9	0.28
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	9	0.28
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	9	0.28
(2,508)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	5	0.28
(2,508)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	5	0.28
(2,508)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	5	0.28
(2,457)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	5	0.28
(2,455)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	1	0.28
(2,222)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	5	0.28
(2,185)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	5	0.28
(2,177)	1:23:A:PRO:HB3	1:25:A:CYS:H	7	0.28
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	5	0.28
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	5	0.28
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	5	0.28
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	8	0.28
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	8	0.28
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	8	0.28
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	9	0.28
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	9	0.28
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	10	0.28
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	10	0.28
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	10	0.28
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	1	0.28
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	1	0.28
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	1	0.28
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	1	0.28
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	1	0.28
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	1	0.28
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	4	0.28
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	4	0.28
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	4	0.28
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	4	0.28
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	4	0.28
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	4	0.28
(2,114)	1:12:A:LEU:H	1:13:A:LYS:HA	9	0.28
(2,107)	1:10:A:GLN:HA	1:11:A:TRP:H	5	0.28
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD21	5	0.28
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD22	5	0.28
(1,606)	1:9:A:ILE:HG13	1:12:A:LEU:HD23	5	0.28
(1,554)	1:4:A:CYS:HA	1:7:A:LEU:HG	7	0.28
(1,537)	1:5:A:VAL:HG11	1:9:A:ILE:H	3	0.28
(1,537)	1:5:A:VAL:HG12	1:9:A:ILE:H	3	0.28
(1,537)	1:5:A:VAL:HG13	1:9:A:ILE:H	3	0.28
(1,537)	1:5:A:VAL:HG11	1:9:A:ILE:H	4	0.28
(1,537)	1:5:A:VAL:HG12	1:9:A:ILE:H	4	0.28
(1,537)	1:5:A:VAL:HG13	1:9:A:ILE:H	4	0.28
(1,523)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	3	0.28
(1,512)	1:23:A:PRO:HA	1:24:A:PRO:HD2	1	0.28
(1,501)	1:12:A:LEU:HA	1:16:A:GLY:HA2	8	0.28
(1,481)	1:7:A:LEU:HA	1:10:A:GLN:HB2	5	0.28
(1,471)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	2	0.28
(1,471)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	6	0.28
(1,469)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	6	0.28
(1,469)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	6	0.28
(1,469)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	6	0.28
(1,420)	1:23:A:PRO:HA	1:23:A:PRO:HD3	7	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	1	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	1	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	2	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	3	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	3	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	5	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	5	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	7	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	7	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	8	0.28
(1,364)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	8	0.28
(1,331)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	1	0.28
(1,331)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	2	0.28
(1,331)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	3	0.28
(1,331)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	4	0.28
(1,331)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	5	0.28
(1,331)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	6	0.28
(1,331)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	7	0.28
(1,331)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	8	0.28
(1,331)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	9	0.28
(1,331)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.28
(1,315)	1:10:A:GLN:HA	1:10:A:GLN:HB2	7	0.28
(1,312)	1:10:A:GLN:HA	1:10:A:GLN:HG2	1	0.28
(1,292)	1:7:A:LEU:HB2	1:7:A:LEU:HG	2	0.28
(1,292)	1:7:A:LEU:HB2	1:7:A:LEU:HG	10	0.28
(1,280)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	2	0.28
(1,280)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	3	0.28
(1,280)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	8	0.28
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG2	4	0.28
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG3	4	0.28
(1,252)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	10	0.28
(1,247)	1:2:A:GLU:HA	1:2:A:GLU:HB3	7	0.28
(1,243)	1:11:A:TRP:HB3	1:12:A:LEU:H	10	0.28
(1,214)	1:15:A:GLY:H	1:16:A:GLY:H	2	0.28
(1,207)	1:8:A:TYR:HD1	1:25:A:CYS:H	9	0.28
(1,207)	1:8:A:TYR:HD2	1:25:A:CYS:H	9	0.28
(1,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	2	0.28
(1,121)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.28
(1,38)	1:21:A:ARG:H	1:21:A:ARG:HB2	9	0.28
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	1	0.27
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	1	0.27
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	1	0.27
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	4	0.27
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	4	0.27
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	6	0.27
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	6	0.27
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	6	0.27
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	6	0.27
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	6	0.27
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	6	0.27
(4,8)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.27
(3,463)	1:8:A:TYR:HA	1:11:A:TRP:HB2	8	0.27
(3,130)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	5	0.27
(3,130)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	5	0.27
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	7	0.27
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG3	10	0.27
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	1	0.27
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	1	0.27
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	1	0.27
(2,493)	1:8:A:TYR:HA	1:11:A:TRP:HB2	8	0.27
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	4	0.27
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	4	0.27
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	4	0.27
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	6	0.27
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	6	0.27
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	6	0.27
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	6	0.27
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	6	0.27
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	6	0.27
(2,139)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	5	0.27
(2,139)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	5	0.27
(2,107)	1:10:A:GLN:HA	1:11:A:TRP:H	10	0.27
(2,22)	1:10:A:GLN:H	1:10:A:GLN:HG2	7	0.27
(2,16)	1:6:A:ARG:H	1:6:A:ARG:HG3	10	0.27
(1,568)	1:19:A:SER:HB3	1:21:A:ARG:HB3	9	0.27
(1,539)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	8	0.27
(1,537)	1:5:A:VAL:HG11	1:9:A:ILE:H	2	0.27
(1,537)	1:5:A:VAL:HG12	1:9:A:ILE:H	2	0.27
(1,537)	1:5:A:VAL:HG13	1:9:A:ILE:H	2	0.27
(1,537)	1:5:A:VAL:HG11	1:9:A:ILE:H	5	0.27
(1,537)	1:5:A:VAL:HG12	1:9:A:ILE:H	5	0.27
(1,537)	1:5:A:VAL:HG13	1:9:A:ILE:H	5	0.27
(1,537)	1:5:A:VAL:HG11	1:9:A:ILE:H	7	0.27
(1,537)	1:5:A:VAL:HG12	1:9:A:ILE:H	7	0.27
(1,537)	1:5:A:VAL:HG13	1:9:A:ILE:H	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:23:A:PRO:HA	1:24:A:PRO:HD2	4	0.27
(1,495)	1:22:A:PRO:HA	1:23:A:PRO:HD3	2	0.27
(1,481)	1:7:A:LEU:HA	1:10:A:GLN:HB2	1	0.27
(1,420)	1:23:A:PRO:HA	1:23:A:PRO:HD3	10	0.27
(1,380)	1:21:A:ARG:HA	1:21:A:ARG:HB2	5	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	1	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	1	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	2	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	2	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	3	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	3	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	4	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	4	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	5	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	5	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	6	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	6	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	7	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	7	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	8	0.27
(1,366)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	8	0.27
(1,355)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	3	0.27
(1,355)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	4	0.27
(1,355)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	5	0.27
(1,355)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	7	0.27
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.27
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.27
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.27
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.27
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.27
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.27
(1,280)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	10	0.27
(1,276)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	9	0.27
(1,274)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	4	0.27
(1,243)	1:11:A:TRP:HB3	1:12:A:LEU:H	8	0.27
(1,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	4	0.27
(1,125)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	9	0.27
(1,92)	1:7:A:LEU:H	1:7:A:LEU:HG	4	0.27
(1,30)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.27
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	5	0.26
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	5	0.26
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	5	0.26
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	5	0.26
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	5	0.26
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	5	0.26
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	5	0.26
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	5	0.26
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	8	0.26
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	8	0.26
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	8	0.26
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	8	0.26
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	8	0.26
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	8	0.26
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	8	0.26
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	8	0.26
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	8	0.26
(4,20)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	6	0.26
(4,20)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	7	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	1	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	1	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	1	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	2	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	2	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	2	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	3	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	3	0.26
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	3	0.26
(4,8)	1:10:A:GLN:HA	1:11:A:TRP:H	1	0.26
(4,8)	1:10:A:GLN:HA	1:11:A:TRP:H	2	0.26
(4,8)	1:10:A:GLN:HA	1:11:A:TRP:H	6	0.26
(4,8)	1:10:A:GLN:HA	1:11:A:TRP:H	8	0.26
(3,485)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	0.26
(3,485)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.26
(3,427)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	4	0.26
(3,427)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	8	0.26
(3,425)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	3	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	2	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	2	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	2	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	5	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	5	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	5	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	6	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	6	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	7	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	7	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	7	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	9	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	9	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	9	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	10	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	10	0.26
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	10	0.26
(3,202)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	10	0.26
(3,177)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	3	0.26
(3,166)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	5	0.26
(3,166)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	5	0.26
(3,141)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	6	0.26
(3,31)	1:4:A:CYS:HB2	1:5:A:VAL:H	5	0.26
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	1	0.26
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	9	0.26
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	5	0.26
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	5	0.26
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	5	0.26
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	5	0.26
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	5	0.26
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	5	0.26
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	5	0.26
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	5	0.26
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	5	0.26
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	8	0.26
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	8	0.26
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	8	0.26
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	8	0.26
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	8	0.26
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	8	0.26
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	8	0.26
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	8	0.26
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	8	0.26
(2,515)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	0.26
(2,515)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.26
(2,457)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	4	0.26
(2,457)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	8	0.26
(2,455)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	2	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	2	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	2	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	5	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	5	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	5	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	6	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	6	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	6	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	7	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	7	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	7	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	9	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	9	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	9	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	10	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	10	0.26
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	10	0.26
(2,222)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	10	0.26
(2,197)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	3	0.26
(2,186)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	5	0.26
(2,186)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	5	0.26
(2,185)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	6	0.26
(2,185)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	7	0.26
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	1	0.26
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	1	0.26
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	1	0.26
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	2	0.26
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	2	0.26
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	2	0.26
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	3	0.26
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	3	0.26
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	3	0.26
(2,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	6	0.26
(2,107)	1:10:A:GLN:HA	1:11:A:TRP:H	1	0.26
(2,107)	1:10:A:GLN:HA	1:11:A:TRP:H	2	0.26
(2,107)	1:10:A:GLN:HA	1:11:A:TRP:H	6	0.26
(2,107)	1:10:A:GLN:HA	1:11:A:TRP:H	8	0.26
(2,35)	1:4:A:CYS:HB2	1:5:A:VAL:H	5	0.26
(2,22)	1:10:A:GLN:H	1:10:A:GLN:HG2	1	0.26
(2,22)	1:10:A:GLN:H	1:10:A:GLN:HG2	9	0.26
(1,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	7	0.26
(1,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	7	0.26
(1,571)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	2	0.26
(1,571)	1:24:A:PRO:HG3	1:25:A:CYS:HB2	2	0.26
(1,571)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	9	0.26
(1,571)	1:24:A:PRO:HG3	1:25:A:CYS:HB2	9	0.26
(1,556)	1:2:A:GLU:HA	1:5:A:VAL:HG11	3	0.26
(1,556)	1:2:A:GLU:HA	1:5:A:VAL:HG12	3	0.26
(1,556)	1:2:A:GLU:HA	1:5:A:VAL:HG13	3	0.26
(1,554)	1:4:A:CYS:HA	1:7:A:LEU:HG	3	0.26
(1,529)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	7	0.26
(1,511)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	1	0.26
(1,508)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	1	0.26
(1,508)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	1	0.26
(1,508)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	1	0.26
(1,501)	1:12:A:LEU:HA	1:16:A:GLY:HA2	6	0.26
(1,495)	1:22:A:PRO:HA	1:23:A:PRO:HD3	3	0.26
(1,495)	1:22:A:PRO:HA	1:23:A:PRO:HD3	4	0.26
(1,469)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	9	0.26
(1,469)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	9	0.26
(1,469)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	9	0.26
(1,438)	1:23:A:PRO:HB2	1:23:A:PRO:HG3	1	0.26
(1,384)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	7	0.26
(1,384)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	9	0.26
(1,355)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	1	0.26
(1,355)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	2	0.26
(1,355)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	6	0.26
(1,355)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	8	0.26
(1,355)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	9	0.26
(1,355)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.26
(1,333)	1:12:A:LEU:HD21	1:12:A:LEU:HG	7	0.26
(1,333)	1:12:A:LEU:HD22	1:12:A:LEU:HG	7	0.26
(1,333)	1:12:A:LEU:HD23	1:12:A:LEU:HG	7	0.26
(1,325)	1:12:A:LEU:HA	1:12:A:LEU:HB3	9	0.26
(1,315)	1:10:A:GLN:HA	1:10:A:GLN:HB2	4	0.26
(1,292)	1:7:A:LEU:HB2	1:7:A:LEU:HG	1	0.26
(1,252)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	8	0.26
(1,247)	1:2:A:GLU:HA	1:2:A:GLU:HB3	8	0.26
(1,174)	1:8:A:TYR:HD1	1:9:A:ILE:HG12	4	0.26
(1,174)	1:8:A:TYR:HD2	1:9:A:ILE:HG12	4	0.26
(1,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	1	0.26
(1,97)	1:12:A:LEU:H	1:12:A:LEU:HG	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:6:A:ARG:HB2	1:7:A:LEU:H	7	0.26
(1,95)	1:6:A:ARG:HB3	1:7:A:LEU:H	7	0.26
(1,55)	1:15:A:GLY:H	1:15:A:GLY:HA2	7	0.26
(1,55)	1:15:A:GLY:H	1:15:A:GLY:HA2	9	0.26
(1,38)	1:21:A:ARG:H	1:21:A:ARG:HB2	2	0.26
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD21	4	0.26
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD22	4	0.26
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD23	4	0.26
(4,20)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	4	0.25
(4,20)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	8	0.25
(4,20)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	9	0.25
(4,20)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	10	0.25
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	6	0.25
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	6	0.25
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	6	0.25
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	7	0.25
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	7	0.25
(4,17)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	7	0.25
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	2	0.25
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	2	0.25
(4,14)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	2	0.25
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	2	0.25
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	2	0.25
(4,14)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	2	0.25
(4,8)	1:10:A:GLN:HA	1:11:A:TRP:H	3	0.25
(3,533)	1:24:A:PRO:HG2	1:25:A:CYS:HB3	6	0.25
(3,533)	1:24:A:PRO:HG3	1:25:A:CYS:HB3	6	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	1	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	1	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	1	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	3	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	3	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	3	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	4	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	4	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	4	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	8	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	8	0.25
(3,308)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	8	0.25
(3,202)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	2	0.25
(3,202)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	8	0.25
(3,177)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,166)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	3	0.25
(3,166)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	3	0.25
(2,565)	1:24:A:PRO:HG2	1:25:A:CYS:HB3	6	0.25
(2,565)	1:24:A:PRO:HG3	1:25:A:CYS:HB3	6	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	1	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	1	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	1	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	3	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	3	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	3	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	4	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	4	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	4	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	8	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	8	0.25
(2,335)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	8	0.25
(2,222)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	2	0.25
(2,222)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	8	0.25
(2,197)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	4	0.25
(2,186)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	3	0.25
(2,186)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	3	0.25
(2,185)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	4	0.25
(2,185)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	8	0.25
(2,185)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	9	0.25
(2,185)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	10	0.25
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	6	0.25
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	6	0.25
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	6	0.25
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	7	0.25
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	7	0.25
(2,172)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	7	0.25
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	2	0.25
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	2	0.25
(2,165)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	2	0.25
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	2	0.25
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	2	0.25
(2,165)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	2	0.25
(2,107)	1:10:A:GLN:HA	1:11:A:TRP:H	3	0.25
(1,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	5	0.25
(1,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	5	0.25
(1,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	5	0.25
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD11	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD12	3	0.25
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD13	3	0.25
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD21	3	0.25
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD22	3	0.25
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD23	3	0.25
(1,489)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	10	0.25
(1,488)	1:8:A:TYR:HA	1:11:A:TRP:HB3	6	0.25
(1,469)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	2	0.25
(1,469)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	2	0.25
(1,469)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	2	0.25
(1,469)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	3	0.25
(1,469)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	3	0.25
(1,469)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	3	0.25
(1,469)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	4	0.25
(1,469)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	4	0.25
(1,469)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	4	0.25
(1,469)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	7	0.25
(1,469)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	7	0.25
(1,469)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	7	0.25
(1,469)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	8	0.25
(1,469)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	8	0.25
(1,469)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	8	0.25
(1,420)	1:23:A:PRO:HA	1:23:A:PRO:HD3	6	0.25
(1,387)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	4	0.25
(1,384)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	1	0.25
(1,376)	1:19:A:SER:HB2	1:19:A:SER:HB3	8	0.25
(1,333)	1:12:A:LEU:HD21	1:12:A:LEU:HG	1	0.25
(1,333)	1:12:A:LEU:HD22	1:12:A:LEU:HG	1	0.25
(1,333)	1:12:A:LEU:HD23	1:12:A:LEU:HG	1	0.25
(1,333)	1:12:A:LEU:HD21	1:12:A:LEU:HG	2	0.25
(1,333)	1:12:A:LEU:HD22	1:12:A:LEU:HG	2	0.25
(1,333)	1:12:A:LEU:HD23	1:12:A:LEU:HG	2	0.25
(1,333)	1:12:A:LEU:HD21	1:12:A:LEU:HG	3	0.25
(1,333)	1:12:A:LEU:HD22	1:12:A:LEU:HG	3	0.25
(1,333)	1:12:A:LEU:HD23	1:12:A:LEU:HG	3	0.25
(1,333)	1:12:A:LEU:HD21	1:12:A:LEU:HG	4	0.25
(1,333)	1:12:A:LEU:HD22	1:12:A:LEU:HG	4	0.25
(1,333)	1:12:A:LEU:HD23	1:12:A:LEU:HG	4	0.25
(1,333)	1:12:A:LEU:HD21	1:12:A:LEU:HG	5	0.25
(1,333)	1:12:A:LEU:HD22	1:12:A:LEU:HG	5	0.25
(1,333)	1:12:A:LEU:HD23	1:12:A:LEU:HG	5	0.25
(1,333)	1:12:A:LEU:HD21	1:12:A:LEU:HG	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:12:A:LEU:HD22	1:12:A:LEU:HG	6	0.25
(1,333)	1:12:A:LEU:HD23	1:12:A:LEU:HG	6	0.25
(1,333)	1:12:A:LEU:HD21	1:12:A:LEU:HG	8	0.25
(1,333)	1:12:A:LEU:HD22	1:12:A:LEU:HG	8	0.25
(1,333)	1:12:A:LEU:HD23	1:12:A:LEU:HG	8	0.25
(1,333)	1:12:A:LEU:HD21	1:12:A:LEU:HG	9	0.25
(1,333)	1:12:A:LEU:HD22	1:12:A:LEU:HG	9	0.25
(1,333)	1:12:A:LEU:HD23	1:12:A:LEU:HG	9	0.25
(1,333)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.25
(1,333)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.25
(1,333)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.25
(1,325)	1:12:A:LEU:HA	1:12:A:LEU:HB3	2	0.25
(1,325)	1:12:A:LEU:HA	1:12:A:LEU:HB3	4	0.25
(1,306)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	1	0.25
(1,306)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	1	0.25
(1,306)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	1	0.25
(1,306)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	2	0.25
(1,306)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	2	0.25
(1,306)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	2	0.25
(1,306)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	6	0.25
(1,306)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	6	0.25
(1,306)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	6	0.25
(1,306)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	8	0.25
(1,306)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	8	0.25
(1,306)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	8	0.25
(1,306)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	9	0.25
(1,306)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	9	0.25
(1,306)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	9	0.25
(1,306)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	10	0.25
(1,306)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	10	0.25
(1,306)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	10	0.25
(1,292)	1:7:A:LEU:HB2	1:7:A:LEU:HG	7	0.25
(1,285)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	9	0.25
(1,285)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.25
(1,280)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	5	0.25
(1,274)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	8	0.25
(1,273)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	7	0.25
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG2	9	0.25
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG3	9	0.25
(1,248)	1:2:A:GLU:HA	1:2:A:GLU:HG2	1	0.25
(1,243)	1:11:A:TRP:HB3	1:12:A:LEU:H	1	0.25
(1,243)	1:11:A:TRP:HB3	1:12:A:LEU:H	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:11:A:TRP:HB3	1:12:A:LEU:H	4	0.25
(1,214)	1:15:A:GLY:H	1:16:A:GLY:H	5	0.25
(1,207)	1:8:A:TYR:HD1	1:25:A:CYS:H	6	0.25
(1,207)	1:8:A:TYR:HD2	1:25:A:CYS:H	6	0.25
(1,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	4	0.25
(1,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	4	0.25
(1,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	7	0.25
(1,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	7	0.25
(1,123)	1:23:A:PRO:HB2	1:25:A:CYS:H	5	0.25
(1,92)	1:7:A:LEU:H	1:7:A:LEU:HG	7	0.25
(1,55)	1:15:A:GLY:H	1:15:A:GLY:HA2	10	0.25
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD21	7	0.25
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD22	7	0.25
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD23	7	0.25
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	9	0.25
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	9	0.25
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	9	0.25
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.25
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.25
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.25
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	3	0.24
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	3	0.24
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	3	0.24
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	3	0.24
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	3	0.24
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	3	0.24
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	3	0.24
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	3	0.24
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	3	0.24
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	7	0.24
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	7	0.24
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	7	0.24
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	7	0.24
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	7	0.24
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	7	0.24
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	7	0.24
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	7	0.24
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	7	0.24
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	2	0.24
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	2	0.24
(4,36)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	2	0.24
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG21	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG22	2	0.24
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG23	2	0.24
(3,202)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	1	0.24
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	3	0.24
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	3	0.24
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	3	0.24
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	3	0.24
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	3	0.24
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	3	0.24
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	3	0.24
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	3	0.24
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	3	0.24
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	7	0.24
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	7	0.24
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	7	0.24
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	7	0.24
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	7	0.24
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	7	0.24
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	7	0.24
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	7	0.24
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	7	0.24
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD11	2	0.24
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD12	2	0.24
(2,611)	1:9:A:ILE:HG12	1:12:A:LEU:HD13	2	0.24
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG21	2	0.24
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG22	2	0.24
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG23	2	0.24
(2,222)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	1	0.24
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	1	0.24
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	1	0.24
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	1	0.24
(1,571)	1:24:A:PRO:HG2	1:25:A:CYS:HB2	3	0.24
(1,571)	1:24:A:PRO:HG3	1:25:A:CYS:HB2	3	0.24
(1,535)	1:9:A:ILE:HA	1:13:A:LYS:H	6	0.24
(1,529)	1:11:A:TRP:HH2	1:23:A:PRO:HG3	6	0.24
(1,512)	1:23:A:PRO:HA	1:24:A:PRO:HD2	9	0.24
(1,511)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	2	0.24
(1,511)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	3	0.24
(1,495)	1:22:A:PRO:HA	1:23:A:PRO:HD3	5	0.24
(1,495)	1:22:A:PRO:HA	1:23:A:PRO:HD3	9	0.24
(1,489)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	9	0.24
(1,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,469)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	5	0.24
(1,469)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	5	0.24
(1,469)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	5	0.24
(1,376)	1:19:A:SER:HB2	1:19:A:SER:HB3	1	0.24
(1,376)	1:19:A:SER:HB2	1:19:A:SER:HB3	2	0.24
(1,376)	1:19:A:SER:HB2	1:19:A:SER:HB3	3	0.24
(1,376)	1:19:A:SER:HB2	1:19:A:SER:HB3	4	0.24
(1,376)	1:19:A:SER:HB2	1:19:A:SER:HB3	5	0.24
(1,376)	1:19:A:SER:HB2	1:19:A:SER:HB3	6	0.24
(1,376)	1:19:A:SER:HB2	1:19:A:SER:HB3	7	0.24
(1,376)	1:19:A:SER:HB2	1:19:A:SER:HB3	9	0.24
(1,376)	1:19:A:SER:HB2	1:19:A:SER:HB3	10	0.24
(1,325)	1:12:A:LEU:HA	1:12:A:LEU:HB3	1	0.24
(1,325)	1:12:A:LEU:HA	1:12:A:LEU:HB3	5	0.24
(1,325)	1:12:A:LEU:HA	1:12:A:LEU:HB3	7	0.24
(1,325)	1:12:A:LEU:HA	1:12:A:LEU:HB3	10	0.24
(1,306)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	3	0.24
(1,306)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	3	0.24
(1,306)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	3	0.24
(1,306)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	4	0.24
(1,306)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	4	0.24
(1,306)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	4	0.24
(1,306)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	5	0.24
(1,306)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	5	0.24
(1,306)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	5	0.24
(1,306)	1:9:A:ILE:HD11	1:9:A:ILE:HG13	7	0.24
(1,306)	1:9:A:ILE:HD12	1:9:A:ILE:HG13	7	0.24
(1,306)	1:9:A:ILE:HD13	1:9:A:ILE:HG13	7	0.24
(1,285)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	1	0.24
(1,285)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	2	0.24
(1,285)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	3	0.24
(1,285)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	4	0.24
(1,285)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	5	0.24
(1,285)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	6	0.24
(1,285)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	7	0.24
(1,285)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	8	0.24
(1,274)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	2	0.24
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG2	3	0.24
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG3	3	0.24
(1,252)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	5	0.24
(1,248)	1:2:A:GLU:HA	1:2:A:GLU:HG2	8	0.24
(1,247)	1:2:A:GLU:HA	1:2:A:GLU:HB3	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.24
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	10	0.24
(1,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	8	0.24
(1,90)	1:10:A:GLN:HB3	1:11:A:TRP:H	9	0.24
(1,75)	1:18:A:SER:HA	1:19:A:SER:H	3	0.24
(1,60)	1:25:A:CYS:H	1:25:A:CYS:HB2	10	0.24
(1,55)	1:15:A:GLY:H	1:15:A:GLY:HA2	4	0.24
(1,55)	1:15:A:GLY:H	1:15:A:GLY:HA2	8	0.24
(1,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.24
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD21	6	0.24
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD22	6	0.24
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD23	6	0.24
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	6	0.24
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	6	0.24
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	6	0.24
(4,20)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	3	0.23
(4,8)	1:10:A:GLN:HA	1:11:A:TRP:H	9	0.23
(4,2)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.23
(3,478)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	3	0.23
(3,478)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	3	0.23
(3,478)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	3	0.23
(3,427)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	2	0.23
(3,202)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	3	0.23
(3,178)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	4	0.23
(3,177)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	2	0.23
(3,143)	1:11:A:TRP:HZ3	1:23:A:PRO:HB2	1	0.23
(2,508)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	3	0.23
(2,508)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	3	0.23
(2,508)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	3	0.23
(2,457)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	2	0.23
(2,222)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	3	0.23
(2,198)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	4	0.23
(2,197)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	2	0.23
(2,185)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	3	0.23
(2,156)	1:11:A:TRP:HZ3	1:23:A:PRO:HB2	1	0.23
(2,107)	1:10:A:GLN:HA	1:11:A:TRP:H	9	0.23
(2,15)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.23
(1,558)	1:2:A:GLU:HA	1:5:A:VAL:HB	8	0.23
(1,512)	1:23:A:PRO:HA	1:24:A:PRO:HD2	8	0.23
(1,511)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	6	0.23
(1,495)	1:22:A:PRO:HA	1:23:A:PRO:HD3	8	0.23
(1,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,469)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	1	0.23
(1,469)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	1	0.23
(1,469)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	1	0.23
(1,469)	1:12:A:LEU:HD11	1:16:A:GLY:HA3	10	0.23
(1,469)	1:12:A:LEU:HD12	1:16:A:GLY:HA3	10	0.23
(1,469)	1:12:A:LEU:HD13	1:16:A:GLY:HA3	10	0.23
(1,465)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	7	0.23
(1,458)	1:25:A:CYS:HA	1:25:A:CYS:HB3	5	0.23
(1,325)	1:12:A:LEU:HA	1:12:A:LEU:HB3	3	0.23
(1,325)	1:12:A:LEU:HA	1:12:A:LEU:HB3	8	0.23
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.23
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.23
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.23
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.23
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.23
(1,289)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.23
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG2	5	0.23
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG3	5	0.23
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG2	7	0.23
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG3	7	0.23
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG2	8	0.23
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG3	8	0.23
(1,252)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	7	0.23
(1,245)	1:11:A:TRP:H	1:12:A:LEU:H	4	0.23
(1,243)	1:11:A:TRP:HB3	1:12:A:LEU:H	3	0.23
(1,243)	1:11:A:TRP:HB3	1:12:A:LEU:H	6	0.23
(1,214)	1:15:A:GLY:H	1:16:A:GLY:H	7	0.23
(1,125)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	7	0.23
(1,60)	1:25:A:CYS:H	1:25:A:CYS:HB2	7	0.23
(1,55)	1:15:A:GLY:H	1:15:A:GLY:HA2	5	0.23
(1,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	6	0.23
(1,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	8	0.23
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD21	1	0.23
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD22	1	0.23
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD23	1	0.23
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	5	0.23
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	5	0.23
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	5	0.23
(4,20)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	2	0.22
(4,19)	1:8:A:TYR:HD1	1:12:A:LEU:HG	4	0.22
(4,19)	1:8:A:TYR:HD2	1:12:A:LEU:HG	4	0.22
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	5	0.22
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	5	0.22
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	5	0.22
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	5	0.22
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	5	0.22
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.22
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.22
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.22
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.22
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.22
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.22
(4,8)	1:10:A:GLN:HA	1:11:A:TRP:H	4	0.22
(4,8)	1:10:A:GLN:HA	1:11:A:TRP:H	7	0.22
(3,485)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	0.22
(3,166)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	8	0.22
(3,166)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	8	0.22
(2,515)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	0.22
(2,186)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	8	0.22
(2,186)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	8	0.22
(2,185)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	2	0.22
(2,184)	1:8:A:TYR:HD1	1:12:A:LEU:HG	4	0.22
(2,184)	1:8:A:TYR:HD2	1:12:A:LEU:HG	4	0.22
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	5	0.22
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	5	0.22
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	5	0.22
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	5	0.22
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	5	0.22
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	5	0.22
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	10	0.22
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	10	0.22
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	10	0.22
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	10	0.22
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	10	0.22
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	10	0.22
(2,107)	1:10:A:GLN:HA	1:11:A:TRP:H	4	0.22
(2,107)	1:10:A:GLN:HA	1:11:A:TRP:H	7	0.22
(1,528)	1:16:A:GLY:H	1:19:A:SER:HB3	3	0.22
(1,512)	1:23:A:PRO:HA	1:24:A:PRO:HD2	7	0.22
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD11	1	0.22
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD12	1	0.22
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD13	1	0.22
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD21	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD22	1	0.22
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD23	1	0.22
(1,495)	1:22:A:PRO:HA	1:23:A:PRO:HD3	7	0.22
(1,488)	1:8:A:TYR:HA	1:11:A:TRP:HB3	3	0.22
(1,482)	1:3:A:GLU:HA	1:6:A:ARG:HB3	4	0.22
(1,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	10	0.22
(1,465)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	6	0.22
(1,292)	1:7:A:LEU:HB2	1:7:A:LEU:HG	4	0.22
(1,292)	1:7:A:LEU:HB2	1:7:A:LEU:HG	5	0.22
(1,259)	1:4:A:CYS:HA	1:4:A:CYS:HB2	3	0.22
(1,259)	1:4:A:CYS:HA	1:4:A:CYS:HB2	6	0.22
(1,252)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	1	0.22
(1,245)	1:11:A:TRP:H	1:12:A:LEU:H	7	0.22
(1,243)	1:11:A:TRP:HB3	1:12:A:LEU:H	7	0.22
(1,214)	1:15:A:GLY:H	1:16:A:GLY:H	8	0.22
(1,207)	1:8:A:TYR:HD1	1:25:A:CYS:H	4	0.22
(1,207)	1:8:A:TYR:HD2	1:25:A:CYS:H	4	0.22
(1,178)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	3	0.22
(1,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.22
(1,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.22
(1,121)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.22
(1,92)	1:7:A:LEU:H	1:7:A:LEU:HG	2	0.22
(1,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.22
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD21	5	0.22
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD22	5	0.22
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD23	5	0.22
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	2	0.22
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	2	0.22
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	2	0.22
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	1	0.21
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	1	0.21
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	1	0.21
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	1	0.21
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	1	0.21
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	1	0.21
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	9	0.21
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	9	0.21
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	9	0.21
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	9	0.21
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	9	0.21
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	9	0.21
(4,20)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	8	0.21
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	8	0.21
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	8	0.21
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	8	0.21
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	8	0.21
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	8	0.21
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	9	0.21
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	9	0.21
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	9	0.21
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	9	0.21
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	9	0.21
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	9	0.21
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.21
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.21
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.21
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.21
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.21
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.21
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.21
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.21
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.21
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.21
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.21
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.21
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.21
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.21
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.21
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.21
(4,2)	1:6:A:ARG:H	1:6:A:ARG:HG2	8	0.21
(3,485)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	6	0.21
(3,178)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	2	0.21
(3,177)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.21
(3,166)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	4	0.21
(3,166)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	4	0.21
(3,37)	1:21:A:ARG:H	1:21:A:ARG:HD3	3	0.21
(2,515)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	6	0.21
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	1	0.21
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	1	0.21
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	1	0.21
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	1	0.21
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	1	0.21
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	9	0.21
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	9	0.21
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	9	0.21
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	9	0.21
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	9	0.21
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	9	0.21
(2,198)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	2	0.21
(2,197)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.21
(2,186)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	4	0.21
(2,186)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	4	0.21
(2,185)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	1	0.21
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	8	0.21
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	8	0.21
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	8	0.21
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	8	0.21
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	8	0.21
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	8	0.21
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	9	0.21
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	9	0.21
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	9	0.21
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	9	0.21
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	9	0.21
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	9	0.21
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.21
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.21
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.21
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.21
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.21
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.21
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.21
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.21
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.21
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.21
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.21
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.21
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.21
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.21
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.21
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.21
(2,41)	1:21:A:ARG:H	1:21:A:ARG:HD3	3	0.21
(2,15)	1:6:A:ARG:H	1:6:A:ARG:HG2	8	0.21
(1,577)	1:11:A:TRP:HB3	1:23:A:PRO:HA	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,558)	1:2:A:GLU:HA	1:5:A:VAL:HB	5	0.21
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	3	0.21
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	3	0.21
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	3	0.21
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	3	0.21
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	3	0.21
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	3	0.21
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	8	0.21
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	8	0.21
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	8	0.21
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	8	0.21
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	8	0.21
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	8	0.21
(1,511)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	8	0.21
(1,488)	1:8:A:TYR:HA	1:11:A:TRP:HB3	7	0.21
(1,465)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	1	0.21
(1,458)	1:25:A:CYS:HA	1:25:A:CYS:HB3	1	0.21
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	1	0.21
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	1	0.21
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	5	0.21
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	5	0.21
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	6	0.21
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	6	0.21
(1,426)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	1	0.21
(1,426)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.21
(1,401)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	7	0.21
(1,387)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	9	0.21
(1,325)	1:12:A:LEU:HA	1:12:A:LEU:HB3	6	0.21
(1,280)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	6	0.21
(1,259)	1:4:A:CYS:HA	1:4:A:CYS:HB2	7	0.21
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG2	10	0.21
(1,255)	1:3:A:GLU:HA	1:3:A:GLU:HG3	10	0.21
(1,252)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	2	0.21
(1,252)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	4	0.21
(1,214)	1:15:A:GLY:H	1:16:A:GLY:H	9	0.21
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	1	0.21
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	1	0.21
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	1	0.21
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	1	0.21
(1,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	6	0.21
(1,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	6	0.21
(1,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	10	0.21
(1,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.21
(1,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.21
(1,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.21
(1,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.21
(1,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.21
(1,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.21
(1,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.21
(1,95)	1:6:A:ARG:HB2	1:7:A:LEU:H	3	0.21
(1,95)	1:6:A:ARG:HB3	1:7:A:LEU:H	3	0.21
(1,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.21
(1,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.21
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD21	3	0.21
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD22	3	0.21
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD23	3	0.21
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD21	10	0.21
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD22	10	0.21
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD23	10	0.21
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	4	0.2
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	4	0.2
(4,37)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	4	0.2
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	4	0.2
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	4	0.2
(4,37)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	4	0.2
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	4	0.2
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	4	0.2
(4,37)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	4	0.2
(4,19)	1:8:A:TYR:HD1	1:12:A:LEU:HG	7	0.2
(4,19)	1:8:A:TYR:HD2	1:12:A:LEU:HG	7	0.2
(4,19)	1:8:A:TYR:HD1	1:12:A:LEU:HG	9	0.2
(4,19)	1:8:A:TYR:HD2	1:12:A:LEU:HG	9	0.2
(4,19)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	0.2
(4,19)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	0.2
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	2	0.2
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	2	0.2
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	2	0.2
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	2	0.2
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	2	0.2
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	2	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.2
(4,10)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.2
(4,10)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.2
(4,2)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.2
(3,359)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	5	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	2	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	2	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	2	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	5	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	5	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	5	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	8	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	8	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	8	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	9	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	9	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	9	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	10	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	10	0.2
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	10	0.2
(3,178)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	1	0.2
(3,143)	1:11:A:TRP:HZ3	1:23:A:PRO:HB2	9	0.2
(3,91)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.2
(3,26)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,26)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.2
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG3	2	0.2
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD11	4	0.2
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD12	4	0.2
(2,618)	1:5:A:VAL:HG21	1:9:A:ILE:HD13	4	0.2
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD11	4	0.2
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD12	4	0.2
(2,618)	1:5:A:VAL:HG22	1:9:A:ILE:HD13	4	0.2
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD11	4	0.2
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD12	4	0.2
(2,618)	1:5:A:VAL:HG23	1:9:A:ILE:HD13	4	0.2
(2,387)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	5	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	2	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	2	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	2	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	5	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	5	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	5	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	8	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	8	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	8	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	9	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	9	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	9	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	10	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	10	0.2
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	10	0.2
(2,198)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	1	0.2
(2,184)	1:8:A:TYR:HD1	1:12:A:LEU:HG	7	0.2
(2,184)	1:8:A:TYR:HD2	1:12:A:LEU:HG	7	0.2
(2,184)	1:8:A:TYR:HD1	1:12:A:LEU:HG	9	0.2
(2,184)	1:8:A:TYR:HD2	1:12:A:LEU:HG	9	0.2
(2,184)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	0.2
(2,184)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	0.2
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	2	0.2
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	2	0.2
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	2	0.2
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	2	0.2
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	2	0.2
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	2	0.2
(2,156)	1:11:A:TRP:HZ3	1:23:A:PRO:HB2	9	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.2
(2,142)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.2
(2,142)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.2
(2,98)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.2
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.2
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.2
(2,16)	1:6:A:ARG:H	1:6:A:ARG:HG3	2	0.2
(2,15)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.2
(1,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	8	0.2
(1,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	8	0.2
(1,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	8	0.2
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	6	0.2
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	6	0.2
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	6	0.2
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	6	0.2
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	6	0.2
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	6	0.2
(1,541)	1:2:A:GLU:HB3	1:6:A:ARG:H	7	0.2
(1,511)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	5	0.2
(1,506)	1:18:A:SER:HB2	1:19:A:SER:H	7	0.2
(1,495)	1:22:A:PRO:HA	1:23:A:PRO:HD3	6	0.2
(1,489)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:7:A:LEU:HA	1:10:A:GLN:HB2	7	0.2
(1,465)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	9	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	2	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	2	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	3	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	3	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	7	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	7	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	9	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	9	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	10	0.2
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	10	0.2
(1,441)	1:24:A:PRO:HA	1:24:A:PRO:HB3	5	0.2
(1,385)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	10	0.2
(1,361)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	8	0.2
(1,315)	1:10:A:GLN:HA	1:10:A:GLN:HB2	5	0.2
(1,292)	1:7:A:LEU:HB2	1:7:A:LEU:HG	3	0.2
(1,292)	1:7:A:LEU:HB2	1:7:A:LEU:HG	6	0.2
(1,259)	1:4:A:CYS:HA	1:4:A:CYS:HB2	8	0.2
(1,254)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	6	0.2
(1,248)	1:2:A:GLU:HA	1:2:A:GLU:HG2	7	0.2
(1,214)	1:15:A:GLY:H	1:16:A:GLY:H	4	0.2
(1,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	9	0.2
(1,175)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	1	0.2
(1,175)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	1	0.2
(1,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	3	0.2
(1,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	6	0.2
(1,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	2	0.2
(1,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	2	0.2
(1,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	9	0.2
(1,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	9	0.2
(1,141)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.2
(1,95)	1:6:A:ARG:HB2	1:7:A:LEU:H	2	0.2
(1,95)	1:6:A:ARG:HB3	1:7:A:LEU:H	2	0.2
(1,55)	1:15:A:GLY:H	1:15:A:GLY:HA2	6	0.2
(1,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.2
(1,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.2
(1,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.2
(1,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.2
(1,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	4	0.2
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	1	0.2
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	1	0.2
(4,25)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	1	0.19
(4,19)	1:8:A:TYR:HD1	1:12:A:LEU:HG	1	0.19
(4,19)	1:8:A:TYR:HD2	1:12:A:LEU:HG	1	0.19
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	6	0.19
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	6	0.19
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	6	0.19
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	6	0.19
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	6	0.19
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	6	0.19
(4,2)	1:6:A:ARG:H	1:6:A:ARG:HG2	5	0.19
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG21	9	0.19
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG22	9	0.19
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG23	9	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	1	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	1	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	1	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	3	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	3	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	3	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	4	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	4	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	4	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	6	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	6	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	6	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	7	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	7	0.19
(3,310)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	7	0.19
(3,177)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	5	0.19
(3,177)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	7	0.19
(3,166)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	6	0.19
(3,166)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	6	0.19
(3,37)	1:21:A:ARG:H	1:21:A:ARG:HD3	2	0.19
(3,37)	1:21:A:ARG:H	1:21:A:ARG:HD3	5	0.19
(3,26)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.19
(3,26)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.19
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG21	9	0.19
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG22	9	0.19
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG23	9	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	1	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	1	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	3	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	3	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	3	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	4	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	4	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	4	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	6	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	6	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	6	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	7	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	7	0.19
(2,338)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	7	0.19
(2,282)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	1	0.19
(2,197)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	5	0.19
(2,197)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	7	0.19
(2,186)	1:8:A:TYR:HE1	1:23:A:PRO:HG2	6	0.19
(2,186)	1:8:A:TYR:HE2	1:23:A:PRO:HG2	6	0.19
(2,184)	1:8:A:TYR:HD1	1:12:A:LEU:HG	1	0.19
(2,184)	1:8:A:TYR:HD2	1:12:A:LEU:HG	1	0.19
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	6	0.19
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	6	0.19
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	6	0.19
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	6	0.19
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	6	0.19
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	6	0.19
(2,41)	1:21:A:ARG:H	1:21:A:ARG:HD3	2	0.19
(2,41)	1:21:A:ARG:H	1:21:A:ARG:HD3	5	0.19
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.19
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.19
(2,15)	1:6:A:ARG:H	1:6:A:ARG:HG2	5	0.19
(1,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	3	0.19
(1,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	3	0.19
(1,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	3	0.19
(1,614)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	4	0.19
(1,614)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	4	0.19
(1,614)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	4	0.19
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	6	0.19
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	6	0.19
(1,567)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	6	0.19
(1,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	7	0.19
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	4	0.19
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	4	0.19
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	4	0.19
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	4	0.19
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	4	0.19
(1,540)	1:2:A:GLU:HB2	1:6:A:ARG:H	4	0.19
(1,511)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	4	0.19
(1,511)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.19
(1,506)	1:18:A:SER:HB2	1:19:A:SER:H	2	0.19
(1,488)	1:8:A:TYR:HA	1:11:A:TRP:HB3	1	0.19
(1,488)	1:8:A:TYR:HA	1:11:A:TRP:HB3	2	0.19
(1,488)	1:8:A:TYR:HA	1:11:A:TRP:HB3	8	0.19
(1,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	9	0.19
(1,460)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	1	0.19
(1,460)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	2	0.19
(1,460)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	3	0.19
(1,460)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	4	0.19
(1,460)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	5	0.19
(1,460)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	6	0.19
(1,460)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	7	0.19
(1,460)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	8	0.19
(1,460)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	9	0.19
(1,460)	1:25:A:CYS:HB2	1:25:A:CYS:HB3	10	0.19
(1,456)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	10	0.19
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	4	0.19
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	4	0.19
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	8	0.19
(1,453)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	8	0.19
(1,452)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	1	0.19
(1,452)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	2	0.19
(1,452)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	3	0.19
(1,452)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	4	0.19
(1,452)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	5	0.19
(1,452)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	6	0.19
(1,452)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	7	0.19
(1,452)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	8	0.19
(1,452)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	9	0.19
(1,452)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	10	0.19
(1,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	1	0.19
(1,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	5	0.19
(1,441)	1:24:A:PRO:HA	1:24:A:PRO:HB3	6	0.19
(1,387)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	8	0.19
(1,374)	1:19:A:SER:HA	1:19:A:SER:HB2	2	0.19
(1,374)	1:19:A:SER:HA	1:19:A:SER:HB2	9	0.19
(1,361)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	1	0.19
(1,361)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	2	0.19
(1,361)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	3	0.19
(1,361)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	4	0.19
(1,361)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	5	0.19
(1,361)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	6	0.19
(1,361)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	7	0.19
(1,361)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	9	0.19
(1,361)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.19
(1,356)	1:17:A:PRO:HA	1:17:A:PRO:HD2	3	0.19
(1,356)	1:17:A:PRO:HA	1:17:A:PRO:HD2	6	0.19
(1,356)	1:17:A:PRO:HA	1:17:A:PRO:HD2	8	0.19
(1,353)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	1	0.19
(1,353)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	2	0.19
(1,353)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	3	0.19
(1,353)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	4	0.19
(1,353)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	5	0.19
(1,353)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	6	0.19
(1,353)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	7	0.19
(1,353)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	8	0.19
(1,353)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	9	0.19
(1,353)	1:14:A:ASP:HB2	1:14:A:ASP:HB3	10	0.19
(1,298)	1:9:A:ILE:HA	1:9:A:ILE:HG13	3	0.19
(1,298)	1:9:A:ILE:HA	1:9:A:ILE:HG13	4	0.19
(1,254)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	1	0.19
(1,254)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	2	0.19
(1,254)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	3	0.19
(1,254)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	4	0.19
(1,254)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	5	0.19
(1,254)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	7	0.19
(1,254)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	8	0.19
(1,254)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	9	0.19
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	9	0.19
(1,192)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	9	0.19
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	5	0.19
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	5	0.19
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	5	0.19
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	5	0.19
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	9	0.19
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	9	0.19
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	9	0.19
(1,155)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.19
(1,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	1	0.19
(1,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	1	0.19
(1,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	8	0.19
(1,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	8	0.19
(1,121)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.19
(1,95)	1:6:A:ARG:HB2	1:7:A:LEU:H	4	0.19
(1,95)	1:6:A:ARG:HB3	1:7:A:LEU:H	4	0.19
(1,95)	1:6:A:ARG:HB2	1:7:A:LEU:H	5	0.19
(1,95)	1:6:A:ARG:HB3	1:7:A:LEU:H	5	0.19
(1,95)	1:6:A:ARG:HB2	1:7:A:LEU:H	6	0.19
(1,95)	1:6:A:ARG:HB3	1:7:A:LEU:H	6	0.19
(1,95)	1:6:A:ARG:HB2	1:7:A:LEU:H	8	0.19
(1,95)	1:6:A:ARG:HB3	1:7:A:LEU:H	8	0.19
(1,92)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.19
(1,90)	1:10:A:GLN:HB3	1:11:A:TRP:H	7	0.19
(1,86)	1:14:A:ASP:H	1:15:A:GLY:H	2	0.19
(1,86)	1:14:A:ASP:H	1:15:A:GLY:H	5	0.19
(1,55)	1:15:A:GLY:H	1:15:A:GLY:HA2	2	0.19
(1,55)	1:15:A:GLY:H	1:15:A:GLY:HA2	3	0.19
(1,38)	1:21:A:ARG:H	1:21:A:ARG:HB2	1	0.19
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD21	8	0.19
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD22	8	0.19
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD23	8	0.19
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD21	9	0.19
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD22	9	0.19
(1,9)	1:9:A:ILE:H	1:12:A:LEU:HD23	9	0.19
(4,25)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	10	0.18
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	2	0.18
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	2	0.18
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	2	0.18
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	2	0.18
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	2	0.18
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	2	0.18
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	4	0.18
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	4	0.18
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	4	0.18
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	4	0.18
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	4	0.18
(4,19)	1:8:A:TYR:HD1	1:12:A:LEU:HG	2	0.18
(4,19)	1:8:A:TYR:HD2	1:12:A:LEU:HG	2	0.18
(4,19)	1:8:A:TYR:HD1	1:12:A:LEU:HG	3	0.18
(4,19)	1:8:A:TYR:HD2	1:12:A:LEU:HG	3	0.18
(4,19)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	0.18
(4,19)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	0.18
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	1	0.18
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	1	0.18
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	1	0.18
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	1	0.18
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	1	0.18
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	1	0.18
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	7	0.18
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	7	0.18
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	7	0.18
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	7	0.18
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	7	0.18
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	7	0.18
(4,2)	1:6:A:ARG:H	1:6:A:ARG:HG2	6	0.18
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	1	0.18
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	1	0.18
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	1	0.18
(3,535)	1:19:A:SER:HB3	1:21:A:ARG:HB3	3	0.18
(3,359)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	2	0.18
(3,178)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	3	0.18
(3,91)	1:7:A:LEU:H	1:10:A:GLN:HB2	3	0.18
(3,26)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.18
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	1	0.18
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	1	0.18
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	1	0.18
(2,568)	1:19:A:SER:HB3	1:21:A:ARG:HB3	3	0.18
(2,387)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	2	0.18
(2,282)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	10	0.18
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	2	0.18
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	2	0.18
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	2	0.18
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	2	0.18
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	2	0.18
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	2	0.18
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	4	0.18
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	4	0.18
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	4	0.18
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	4	0.18
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	4	0.18
(2,198)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	3	0.18
(2,184)	1:8:A:TYR:HD1	1:12:A:LEU:HG	2	0.18
(2,184)	1:8:A:TYR:HD2	1:12:A:LEU:HG	2	0.18
(2,184)	1:8:A:TYR:HD1	1:12:A:LEU:HG	3	0.18
(2,184)	1:8:A:TYR:HD2	1:12:A:LEU:HG	3	0.18
(2,184)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	0.18
(2,184)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	0.18
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	1	0.18
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	1	0.18
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	1	0.18
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	1	0.18
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	1	0.18
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	1	0.18
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	7	0.18
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	7	0.18
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	7	0.18
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	7	0.18
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	7	0.18
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	7	0.18
(2,98)	1:7:A:LEU:H	1:10:A:GLN:HB2	3	0.18
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.18
(2,15)	1:6:A:ARG:H	1:6:A:ARG:HG2	6	0.18
(1,555)	1:2:A:GLU:HA	1:5:A:VAL:HG21	3	0.18
(1,555)	1:2:A:GLU:HA	1:5:A:VAL:HG22	3	0.18
(1,555)	1:2:A:GLU:HA	1:5:A:VAL:HG23	3	0.18
(1,548)	1:12:A:LEU:H	1:14:A:ASP:H	10	0.18
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	1	0.18
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	1	0.18
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	1	0.18
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	1	0.18
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	1	0.18
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	1	0.18
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	7	0.18
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	7	0.18
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	7	0.18
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	7	0.18
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	7	0.18
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:11:A:TRP:HE3	1:23:A:PRO:HB3	3	0.18
(1,490)	1:14:A:ASP:HB3	1:19:A:SER:HB2	7	0.18
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	6	0.18
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	6	0.18
(1,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	6	0.18
(1,441)	1:24:A:PRO:HA	1:24:A:PRO:HB3	1	0.18
(1,441)	1:24:A:PRO:HA	1:24:A:PRO:HB3	8	0.18
(1,387)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	1	0.18
(1,374)	1:19:A:SER:HA	1:19:A:SER:HB2	4	0.18
(1,374)	1:19:A:SER:HA	1:19:A:SER:HB2	8	0.18
(1,374)	1:19:A:SER:HA	1:19:A:SER:HB2	10	0.18
(1,356)	1:17:A:PRO:HA	1:17:A:PRO:HD2	1	0.18
(1,356)	1:17:A:PRO:HA	1:17:A:PRO:HD2	2	0.18
(1,356)	1:17:A:PRO:HA	1:17:A:PRO:HD2	4	0.18
(1,356)	1:17:A:PRO:HA	1:17:A:PRO:HD2	5	0.18
(1,356)	1:17:A:PRO:HA	1:17:A:PRO:HD2	7	0.18
(1,315)	1:10:A:GLN:HA	1:10:A:GLN:HB2	10	0.18
(1,312)	1:10:A:GLN:HA	1:10:A:GLN:HG2	7	0.18
(1,312)	1:10:A:GLN:HA	1:10:A:GLN:HG2	9	0.18
(1,298)	1:9:A:ILE:HA	1:9:A:ILE:HG13	2	0.18
(1,298)	1:9:A:ILE:HA	1:9:A:ILE:HG13	7	0.18
(1,293)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	2	0.18
(1,293)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	4	0.18
(1,293)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	7	0.18
(1,293)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.18
(1,274)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	3	0.18
(1,260)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	2	0.18
(1,260)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	3	0.18
(1,260)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	4	0.18
(1,260)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	7	0.18
(1,260)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	9	0.18
(1,260)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	10	0.18
(1,254)	1:2:A:GLU:HB2	1:2:A:GLU:HB3	10	0.18
(1,249)	1:2:A:GLU:HA	1:2:A:GLU:HG3	3	0.18
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	3	0.18
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	3	0.18
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	3	0.18
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	3	0.18
(1,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	5	0.18
(1,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	5	0.18
(1,121)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.18
(1,121)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:7:A:LEU:H	1:7:A:LEU:HB2	5	0.18
(1,92)	1:7:A:LEU:H	1:7:A:LEU:HG	3	0.18
(1,92)	1:7:A:LEU:H	1:7:A:LEU:HG	5	0.18
(1,92)	1:7:A:LEU:H	1:7:A:LEU:HG	6	0.18
(4,25)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	7	0.17
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	5	0.17
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	5	0.17
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	5	0.17
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	5	0.17
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	5	0.17
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	5	0.17
(4,19)	1:8:A:TYR:HD1	1:12:A:LEU:HG	6	0.17
(4,19)	1:8:A:TYR:HD2	1:12:A:LEU:HG	6	0.17
(4,19)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	0.17
(4,19)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	0.17
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	3	0.17
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	3	0.17
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	3	0.17
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	3	0.17
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	3	0.17
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	3	0.17
(3,388)	1:23:A:PRO:HA	1:23:A:PRO:HG3	6	0.17
(3,181)	1:15:A:GLY:HA3	1:16:A:GLY:H	7	0.17
(3,91)	1:7:A:LEU:H	1:10:A:GLN:HB2	6	0.17
(2,416)	1:23:A:PRO:HA	1:23:A:PRO:HG3	6	0.17
(2,282)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	7	0.17
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	5	0.17
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	5	0.17
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	5	0.17
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	5	0.17
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	5	0.17
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	5	0.17
(2,201)	1:15:A:GLY:HA3	1:16:A:GLY:H	7	0.17
(2,184)	1:8:A:TYR:HD1	1:12:A:LEU:HG	6	0.17
(2,184)	1:8:A:TYR:HD2	1:12:A:LEU:HG	6	0.17
(2,184)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	0.17
(2,184)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	0.17
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	3	0.17
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	3	0.17
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	3	0.17
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	3	0.17
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	3	0.17
(2,98)	1:7:A:LEU:H	1:10:A:GLN:HB2	6	0.17
(1,581)	1:1:A:GLU:HB3	1:2:A:GLU:HG2	7	0.17
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	4	0.17
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	4	0.17
(1,565)	1:24:A:PRO:HG2	1:25:A:CYS:HB3	4	0.17
(1,565)	1:24:A:PRO:HG3	1:25:A:CYS:HB3	4	0.17
(1,559)	1:19:A:SER:HB2	1:21:A:ARG:HB2	7	0.17
(1,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	0.17
(1,511)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	7	0.17
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD11	9	0.17
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD12	9	0.17
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD13	9	0.17
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD21	9	0.17
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD22	9	0.17
(1,496)	1:4:A:CYS:HA	1:7:A:LEU:HD23	9	0.17
(1,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	2	0.17
(1,474)	1:22:A:PRO:HB2	1:23:A:PRO:HD3	5	0.17
(1,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	2	0.17
(1,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	7	0.17
(1,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	10	0.17
(1,441)	1:24:A:PRO:HA	1:24:A:PRO:HB3	2	0.17
(1,441)	1:24:A:PRO:HA	1:24:A:PRO:HB3	3	0.17
(1,441)	1:24:A:PRO:HA	1:24:A:PRO:HB3	9	0.17
(1,441)	1:24:A:PRO:HA	1:24:A:PRO:HB3	10	0.17
(1,298)	1:9:A:ILE:HA	1:9:A:ILE:HG13	1	0.17
(1,298)	1:9:A:ILE:HA	1:9:A:ILE:HG13	6	0.17
(1,298)	1:9:A:ILE:HA	1:9:A:ILE:HG13	10	0.17
(1,293)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	1	0.17
(1,293)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	3	0.17
(1,293)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	5	0.17
(1,293)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	6	0.17
(1,293)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	8	0.17
(1,293)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	9	0.17
(1,292)	1:7:A:LEU:HB2	1:7:A:LEU:HG	9	0.17
(1,260)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	1	0.17
(1,260)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	5	0.17
(1,260)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	6	0.17
(1,260)	1:4:A:CYS:HB2	1:4:A:CYS:HB3	8	0.17
(1,214)	1:15:A:GLY:H	1:16:A:GLY:H	6	0.17
(1,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	5	0.17
(1,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	9	0.17
(1,125)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	2	0.17
(1,92)	1:7:A:LEU:H	1:7:A:LEU:HG	1	0.17
(1,86)	1:14:A:ASP:H	1:15:A:GLY:H	6	0.17
(1,86)	1:14:A:ASP:H	1:15:A:GLY:H	7	0.17
(1,55)	1:15:A:GLY:H	1:15:A:GLY:HA2	1	0.17
(1,51)	1:20:A:GLY:H	1:20:A:GLY:HA2	2	0.17
(1,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.17
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	3	0.16
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	3	0.16
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	3	0.16
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	3	0.16
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	3	0.16
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	3	0.16
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	4	0.16
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	4	0.16
(4,16)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	4	0.16
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	4	0.16
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	4	0.16
(4,16)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	4	0.16
(4,3)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.16
(3,388)	1:23:A:PRO:HA	1:23:A:PRO:HG3	7	0.16
(3,201)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	5	0.16
(3,178)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	5	0.16
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG3	4	0.16
(2,416)	1:23:A:PRO:HA	1:23:A:PRO:HG3	7	0.16
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	3	0.16
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	3	0.16
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	3	0.16
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	3	0.16
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	3	0.16
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	3	0.16
(2,221)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	5	0.16
(2,198)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	5	0.16
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD11	4	0.16
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD12	4	0.16
(2,169)	1:8:A:TYR:HE1	1:9:A:ILE:HD13	4	0.16
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD11	4	0.16
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD12	4	0.16
(2,169)	1:8:A:TYR:HE2	1:9:A:ILE:HD13	4	0.16
(2,23)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.16
(2,16)	1:6:A:ARG:H	1:6:A:ARG:HG3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG11	10	0.16
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG12	10	0.16
(1,588)	1:2:A:GLU:HG2	1:5:A:VAL:HG13	10	0.16
(1,568)	1:19:A:SER:HB3	1:21:A:ARG:HB3	10	0.16
(1,567)	1:22:A:PRO:HB3	1:23:A:PRO:HD2	7	0.16
(1,553)	1:22:A:PRO:HA	1:23:A:PRO:HG2	2	0.16
(1,553)	1:22:A:PRO:HA	1:23:A:PRO:HG2	9	0.16
(1,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	1	0.16
(1,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	2	0.16
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	10	0.16
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	10	0.16
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	10	0.16
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	10	0.16
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	10	0.16
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	10	0.16
(1,489)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	2	0.16
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	4	0.16
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	4	0.16
(1,458)	1:25:A:CYS:HA	1:25:A:CYS:HB3	10	0.16
(1,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	8	0.16
(1,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	9	0.16
(1,441)	1:24:A:PRO:HA	1:24:A:PRO:HB3	4	0.16
(1,441)	1:24:A:PRO:HA	1:24:A:PRO:HB3	7	0.16
(1,399)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	1	0.16
(1,399)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	2	0.16
(1,399)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	3	0.16
(1,399)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	4	0.16
(1,399)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	5	0.16
(1,399)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	6	0.16
(1,399)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	7	0.16
(1,399)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	8	0.16
(1,399)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	9	0.16
(1,399)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	10	0.16
(1,374)	1:19:A:SER:HA	1:19:A:SER:HB2	5	0.16
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	1	0.16
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	1	0.16
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	1	0.16
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	1	0.16
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	1	0.16
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	1	0.16
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	1	0.16
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	1	0.16
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	2	0.16
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	2	0.16
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	2	0.16
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	2	0.16
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	2	0.16
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	2	0.16
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	2	0.16
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	2	0.16
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	2	0.16
(1,298)	1:9:A:ILE:HA	1:9:A:ILE:HG13	5	0.16
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	9	0.16
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	9	0.16
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	9	0.16
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	9	0.16
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	9	0.16
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	9	0.16
(1,259)	1:4:A:CYS:HA	1:4:A:CYS:HB2	2	0.16
(1,252)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	9	0.16
(1,245)	1:11:A:TRP:H	1:12:A:LEU:H	9	0.16
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	2	0.16
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	2	0.16
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	2	0.16
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	2	0.16
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG2	3	0.16
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	3	0.16
(1,151)	1:8:A:TYR:HD1	1:24:A:PRO:HD3	3	0.16
(1,151)	1:8:A:TYR:HD2	1:24:A:PRO:HD3	3	0.16
(1,140)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	3	0.16
(1,140)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	7	0.16
(1,140)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	8	0.16
(1,140)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	9	0.16
(1,125)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	5	0.16
(1,86)	1:14:A:ASP:H	1:15:A:GLY:H	9	0.16
(1,51)	1:20:A:GLY:H	1:20:A:GLY:HA2	4	0.16
(1,51)	1:20:A:GLY:H	1:20:A:GLY:HA2	9	0.16
(1,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.16
(1,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.16
(1,42)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.16
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	7	0.15
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	7	0.15
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	7	0.15
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	7	0.15
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	7	0.15
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	10	0.15
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	10	0.15
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	10	0.15
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	10	0.15
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	10	0.15
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	10	0.15
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	2	0.15
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	2	0.15
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	2	0.15
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	4	0.15
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	4	0.15
(3,557)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	4	0.15
(3,427)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	9	0.15
(3,359)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	3	0.15
(3,205)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	5	0.15
(3,205)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	9	0.15
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.15
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG3	3	0.15
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	2	0.15
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	2	0.15
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	2	0.15
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD11	4	0.15
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD12	4	0.15
(2,591)	1:2:A:GLU:HG2	1:9:A:ILE:HD13	4	0.15
(2,457)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	9	0.15
(2,387)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	3	0.15
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	7	0.15
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	7	0.15
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	7	0.15
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	7	0.15
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	7	0.15
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	7	0.15
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	10	0.15
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	10	0.15
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	10	0.15
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	10	0.15
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	10	0.15
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	10	0.15
(2,225)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,225)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	9	0.15
(2,22)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.15
(2,16)	1:6:A:ARG:H	1:6:A:ARG:HG3	3	0.15
(1,621)	1:7:A:LEU:HB3	1:24:A:PRO:HG2	8	0.15
(1,621)	1:7:A:LEU:HB3	1:24:A:PRO:HG3	8	0.15
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	10	0.15
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	10	0.15
(1,558)	1:2:A:GLU:HA	1:5:A:VAL:HB	2	0.15
(1,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	0.15
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	9	0.15
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	9	0.15
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	9	0.15
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	9	0.15
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	9	0.15
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	9	0.15
(1,489)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	1	0.15
(1,488)	1:8:A:TYR:HA	1:11:A:TRP:HB3	10	0.15
(1,465)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	2	0.15
(1,458)	1:25:A:CYS:HA	1:25:A:CYS:HB3	8	0.15
(1,458)	1:25:A:CYS:HA	1:25:A:CYS:HB3	9	0.15
(1,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	3	0.15
(1,447)	1:24:A:PRO:HB3	1:24:A:PRO:HD2	4	0.15
(1,390)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	2	0.15
(1,390)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	3	0.15
(1,390)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	4	0.15
(1,390)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	5	0.15
(1,390)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	10	0.15
(1,384)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	8	0.15
(1,374)	1:19:A:SER:HA	1:19:A:SER:HB2	1	0.15
(1,374)	1:19:A:SER:HA	1:19:A:SER:HB2	6	0.15
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	4	0.15
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	4	0.15
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	4	0.15
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	4	0.15
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	4	0.15
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	4	0.15
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	4	0.15
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	4	0.15
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	4	0.15
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	7	0.15
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	7	0.15
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	7	0.15
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	7	0.15
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	7	0.15
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	7	0.15
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	7	0.15
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	7	0.15
(1,298)	1:9:A:ILE:HA	1:9:A:ILE:HG13	8	0.15
(1,247)	1:2:A:GLU:HA	1:2:A:GLU:HB3	10	0.15
(1,157)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	2	0.15
(1,157)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	2	0.15
(1,140)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	2	0.15
(1,140)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	5	0.15
(1,140)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	6	0.15
(1,125)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	4	0.15
(1,108)	1:19:A:SER:HB2	1:21:A:ARG:H	3	0.15
(1,95)	1:6:A:ARG:HB2	1:7:A:LEU:H	1	0.15
(1,95)	1:6:A:ARG:HB3	1:7:A:LEU:H	1	0.15
(1,86)	1:14:A:ASP:H	1:15:A:GLY:H	1	0.15
(1,86)	1:14:A:ASP:H	1:15:A:GLY:H	3	0.15
(1,86)	1:14:A:ASP:H	1:15:A:GLY:H	4	0.15
(1,51)	1:20:A:GLY:H	1:20:A:GLY:HA2	1	0.15
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD11	1	0.14
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD12	1	0.14
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD13	1	0.14
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD11	7	0.14
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD12	7	0.14
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD13	7	0.14
(3,205)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	2	0.14
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	2	0.14
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG3	6	0.14
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD11	1	0.14
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD12	1	0.14
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD13	1	0.14
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD11	7	0.14
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD12	7	0.14
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD13	7	0.14
(2,225)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	2	0.14
(2,22)	1:10:A:GLN:H	1:10:A:GLN:HG2	2	0.14
(2,16)	1:6:A:ARG:H	1:6:A:ARG:HG3	6	0.14
(1,553)	1:22:A:PRO:HA	1:23:A:PRO:HG2	1	0.14
(1,553)	1:22:A:PRO:HA	1:23:A:PRO:HG2	4	0.14
(1,553)	1:22:A:PRO:HA	1:23:A:PRO:HG2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:12:A:LEU:H	1:14:A:ASP:H	1	0.14
(1,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	0.14
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	5	0.14
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	5	0.14
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	5	0.14
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	5	0.14
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	5	0.14
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	5	0.14
(1,518)	1:1:A:GLU:HA	1:1:A:GLU:HB2	9	0.14
(1,489)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	3	0.14
(1,489)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	4	0.14
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	10	0.14
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	10	0.14
(1,458)	1:25:A:CYS:HA	1:25:A:CYS:HB3	3	0.14
(1,445)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	4	0.14
(1,445)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	6	0.14
(1,445)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	7	0.14
(1,445)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	9	0.14
(1,445)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	10	0.14
(1,426)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	3	0.14
(1,426)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	6	0.14
(1,426)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	7	0.14
(1,426)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	9	0.14
(1,390)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	1	0.14
(1,390)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	8	0.14
(1,390)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	9	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	3	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	3	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	3	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	3	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	3	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	3	0.14
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	3	0.14
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	3	0.14
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	3	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	6	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	6	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	6	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	6	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	6	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	6	0.14
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	6	0.14
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	6	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	8	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	8	0.14
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	8	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	8	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	8	0.14
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	8	0.14
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	8	0.14
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	8	0.14
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	8	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	3	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	3	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	3	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	3	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	3	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	3	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	6	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	6	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	6	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	6	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	6	0.14
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	6	0.14
(1,274)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	5	0.14
(1,267)	1:6:A:ARG:HA	1:6:A:ARG:HD3	9	0.14
(1,259)	1:4:A:CYS:HA	1:4:A:CYS:HB2	9	0.14
(1,241)	1:12:A:LEU:HA	1:16:A:GLY:H	7	0.14
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG2	10	0.14
(1,180)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	10	0.14
(1,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	2	0.14
(1,179)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	4	0.14
(1,140)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	1	0.14
(1,108)	1:19:A:SER:HB2	1:21:A:ARG:H	7	0.14
(1,86)	1:14:A:ASP:H	1:15:A:GLY:H	10	0.14
(1,65)	1:19:A:SER:H	1:19:A:SER:HB3	2	0.14
(1,65)	1:19:A:SER:H	1:19:A:SER:HB3	9	0.14
(1,64)	1:19:A:SER:H	1:19:A:SER:HB2	1	0.14
(1,64)	1:19:A:SER:H	1:19:A:SER:HB2	5	0.14
(1,51)	1:20:A:GLY:H	1:20:A:GLY:HA2	3	0.14
(1,51)	1:20:A:GLY:H	1:20:A:GLY:HA2	5	0.14
(1,51)	1:20:A:GLY:H	1:20:A:GLY:HA2	6	0.14
(1,51)	1:20:A:GLY:H	1:20:A:GLY:HA2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:20:A:GLY:H	1:20:A:GLY:HA2	8	0.14
(1,50)	1:9:A:ILE:H	1:9:A:ILE:HB	2	0.14
(1,50)	1:9:A:ILE:H	1:9:A:ILE:HB	7	0.14
(1,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	0.14
(1,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	2	0.14
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	8	0.13
(4,24)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	8	0.13
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	8	0.13
(4,24)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	8	0.13
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	8	0.13
(4,24)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	8	0.13
(4,3)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.13
(3,246)	1:6:A:ARG:HA	1:6:A:ARG:HG2	9	0.13
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG3	5	0.13
(2,270)	1:6:A:ARG:HA	1:6:A:ARG:HG2	9	0.13
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	8	0.13
(2,238)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	8	0.13
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	8	0.13
(2,238)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	8	0.13
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	8	0.13
(2,238)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	8	0.13
(2,23)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.13
(2,16)	1:6:A:ARG:H	1:6:A:ARG:HG3	5	0.13
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	1	0.13
(1,569)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	1	0.13
(1,553)	1:22:A:PRO:HA	1:23:A:PRO:HG2	3	0.13
(1,509)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	3	0.13
(1,509)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	5	0.13
(1,507)	1:11:A:TRP:HA	1:14:A:ASP:HB3	6	0.13
(1,489)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	7	0.13
(1,488)	1:8:A:TYR:HA	1:11:A:TRP:HB3	4	0.13
(1,458)	1:25:A:CYS:HA	1:25:A:CYS:HB3	2	0.13
(1,445)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	1	0.13
(1,445)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	2	0.13
(1,445)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	3	0.13
(1,445)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	5	0.13
(1,445)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	8	0.13
(1,426)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	2	0.13
(1,426)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	4	0.13
(1,426)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	5	0.13
(1,426)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	8	0.13
(1,401)	1:22:A:PRO:HB2	1:22:A:PRO:HD2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	6	0.13
(1,390)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	7	0.13
(1,380)	1:21:A:ARG:HA	1:21:A:ARG:HB2	10	0.13
(1,368)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	9	0.13
(1,368)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	9	0.13
(1,359)	1:17:A:PRO:HA	1:17:A:PRO:HG2	6	0.13
(1,359)	1:17:A:PRO:HA	1:17:A:PRO:HG3	6	0.13
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	5	0.13
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	5	0.13
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	5	0.13
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	5	0.13
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	5	0.13
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	5	0.13
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	5	0.13
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	5	0.13
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	5	0.13
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	9	0.13
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	9	0.13
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	9	0.13
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	9	0.13
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	9	0.13
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	9	0.13
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	9	0.13
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	9	0.13
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	9	0.13
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD21	10	0.13
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD22	10	0.13
(1,339)	1:12:A:LEU:HD11	1:12:A:LEU:HD23	10	0.13
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD21	10	0.13
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD22	10	0.13
(1,339)	1:12:A:LEU:HD12	1:12:A:LEU:HD23	10	0.13
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD21	10	0.13
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD22	10	0.13
(1,339)	1:12:A:LEU:HD13	1:12:A:LEU:HD23	10	0.13
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	4	0.13
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	4	0.13
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	4	0.13
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	5	0.13
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	5	0.13
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	5	0.13
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	5	0.13
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	5	0.13
(1,251)	1:2:A:GLU:HB3	1:2:A:GLU:HG2	3	0.13
(1,140)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	4	0.13
(1,140)	1:11:A:TRP:HB2	1:11:A:TRP:HD1	10	0.13
(1,125)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	3	0.13
(1,86)	1:14:A:ASP:H	1:15:A:GLY:H	8	0.13
(1,64)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.13
(1,51)	1:20:A:GLY:H	1:20:A:GLY:HA2	10	0.13
(1,50)	1:9:A:ILE:H	1:9:A:ILE:HB	1	0.13
(1,50)	1:9:A:ILE:H	1:9:A:ILE:HB	3	0.13
(1,50)	1:9:A:ILE:H	1:9:A:ILE:HB	8	0.13
(1,50)	1:9:A:ILE:H	1:9:A:ILE:HB	10	0.13
(1,47)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.13
(1,37)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	10	0.13
(4,3)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD11	4	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD12	4	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD13	4	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD11	6	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD12	6	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD13	6	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD11	10	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD12	10	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD13	10	0.12
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG21	8	0.12
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG22	8	0.12
(3,555)	1:2:A:GLU:HG2	1:5:A:VAL:HG23	8	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD11	3	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD12	3	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD13	3	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD11	4	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD12	4	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD13	4	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD11	6	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD12	6	0.12
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD13	6	0.12
(3,257)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	6	0.12
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	8	0.12
(3,14)	1:6:A:ARG:H	1:6:A:ARG:HG3	8	0.12
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG11	6	0.12
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG12	6	0.12
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG13	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG11	9	0.12
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG12	9	0.12
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG13	9	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD11	4	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD12	4	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD13	4	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD11	6	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD12	6	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD13	6	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD11	10	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD12	10	0.12
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD13	10	0.12
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG21	8	0.12
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG22	8	0.12
(2,589)	1:2:A:GLU:HG2	1:5:A:VAL:HG23	8	0.12
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD11	3	0.12
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD12	3	0.12
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD13	3	0.12
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD11	4	0.12
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD12	4	0.12
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD13	4	0.12
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD11	6	0.12
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD12	6	0.12
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD13	6	0.12
(2,281)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	6	0.12
(2,23)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.12
(2,22)	1:10:A:GLN:H	1:10:A:GLN:HG2	8	0.12
(2,16)	1:6:A:ARG:H	1:6:A:ARG:HG3	8	0.12
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG11	6	0.12
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG12	6	0.12
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG13	6	0.12
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG11	9	0.12
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG12	9	0.12
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG13	9	0.12
(1,570)	1:24:A:PRO:HB2	1:25:A:CYS:HB2	7	0.12
(1,553)	1:22:A:PRO:HA	1:23:A:PRO:HG2	5	0.12
(1,548)	1:12:A:LEU:H	1:14:A:ASP:H	8	0.12
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	2	0.12
(1,544)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	2	0.12
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	2	0.12
(1,544)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	2	0.12
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	2	0.12
(1,518)	1:1:A:GLU:HA	1:1:A:GLU:HB2	2	0.12
(1,509)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	1	0.12
(1,509)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	2	0.12
(1,509)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	4	0.12
(1,509)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	6	0.12
(1,509)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	7	0.12
(1,509)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	8	0.12
(1,509)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	9	0.12
(1,509)	1:23:A:PRO:HD2	1:23:A:PRO:HD3	10	0.12
(1,408)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	3	0.12
(1,408)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	10	0.12
(1,385)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	3	0.12
(1,368)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	10	0.12
(1,368)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	10	0.12
(1,359)	1:17:A:PRO:HA	1:17:A:PRO:HG2	7	0.12
(1,359)	1:17:A:PRO:HA	1:17:A:PRO:HG3	7	0.12
(1,334)	1:12:A:LEU:HD11	1:12:A:LEU:HG	2	0.12
(1,334)	1:12:A:LEU:HD12	1:12:A:LEU:HG	2	0.12
(1,334)	1:12:A:LEU:HD13	1:12:A:LEU:HG	2	0.12
(1,334)	1:12:A:LEU:HD11	1:12:A:LEU:HG	3	0.12
(1,334)	1:12:A:LEU:HD12	1:12:A:LEU:HG	3	0.12
(1,334)	1:12:A:LEU:HD13	1:12:A:LEU:HG	3	0.12
(1,334)	1:12:A:LEU:HD11	1:12:A:LEU:HG	4	0.12
(1,334)	1:12:A:LEU:HD12	1:12:A:LEU:HG	4	0.12
(1,334)	1:12:A:LEU:HD13	1:12:A:LEU:HG	4	0.12
(1,334)	1:12:A:LEU:HD11	1:12:A:LEU:HG	5	0.12
(1,334)	1:12:A:LEU:HD12	1:12:A:LEU:HG	5	0.12
(1,334)	1:12:A:LEU:HD13	1:12:A:LEU:HG	5	0.12
(1,334)	1:12:A:LEU:HD11	1:12:A:LEU:HG	6	0.12
(1,334)	1:12:A:LEU:HD12	1:12:A:LEU:HG	6	0.12
(1,334)	1:12:A:LEU:HD13	1:12:A:LEU:HG	6	0.12
(1,334)	1:12:A:LEU:HD11	1:12:A:LEU:HG	7	0.12
(1,334)	1:12:A:LEU:HD12	1:12:A:LEU:HG	7	0.12
(1,334)	1:12:A:LEU:HD13	1:12:A:LEU:HG	7	0.12
(1,334)	1:12:A:LEU:HD11	1:12:A:LEU:HG	8	0.12
(1,334)	1:12:A:LEU:HD12	1:12:A:LEU:HG	8	0.12
(1,334)	1:12:A:LEU:HD13	1:12:A:LEU:HG	8	0.12
(1,334)	1:12:A:LEU:HD11	1:12:A:LEU:HG	9	0.12
(1,334)	1:12:A:LEU:HD12	1:12:A:LEU:HG	9	0.12
(1,334)	1:12:A:LEU:HD13	1:12:A:LEU:HG	9	0.12
(1,334)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.12
(1,334)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.12
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	3	0.12
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	3	0.12
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	3	0.12
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	4	0.12
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	4	0.12
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	4	0.12
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	4	0.12
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	4	0.12
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	4	0.12
(1,251)	1:2:A:GLU:HB3	1:2:A:GLU:HG2	6	0.12
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG2	8	0.12
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG2	8	0.12
(1,187)	1:8:A:TYR:HD1	1:24:A:PRO:HG3	8	0.12
(1,187)	1:8:A:TYR:HD2	1:24:A:PRO:HG3	8	0.12
(1,130)	1:5:A:VAL:HA	1:8:A:TYR:HD1	5	0.12
(1,130)	1:5:A:VAL:HA	1:8:A:TYR:HD2	5	0.12
(1,92)	1:7:A:LEU:H	1:7:A:LEU:HG	9	0.12
(1,80)	1:13:A:LYS:H	1:13:A:LYS:HB2	9	0.12
(1,80)	1:13:A:LYS:H	1:13:A:LYS:HB3	9	0.12
(1,50)	1:9:A:ILE:H	1:9:A:ILE:HB	4	0.12
(1,50)	1:9:A:ILE:H	1:9:A:ILE:HB	5	0.12
(1,50)	1:9:A:ILE:H	1:9:A:ILE:HB	6	0.12
(1,50)	1:9:A:ILE:H	1:9:A:ILE:HB	9	0.12
(1,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.12
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	3	0.12
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	3	0.12
(1,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	3	0.12
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD11	7	0.11
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD12	7	0.11
(3,563)	1:2:A:GLU:HB2	1:9:A:ILE:HD13	7	0.11
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD11	5	0.11
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD12	5	0.11
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD13	5	0.11
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD11	8	0.11
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD12	8	0.11
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD13	8	0.11
(3,455)	1:11:A:TRP:HA	1:14:A:ASP:HB2	7	0.11
(3,425)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	6	0.11
(3,425)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	7	0.11
(3,257)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,257)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	4	0.11
(3,257)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	5	0.11
(3,205)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	1	0.11
(3,201)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	2	0.11
(3,181)	1:15:A:GLY:HA3	1:16:A:GLY:H	9	0.11
(3,160)	1:23:A:PRO:HB3	1:25:A:CYS:H	1	0.11
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG11	2	0.11
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG12	2	0.11
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG13	2	0.11
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG11	10	0.11
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG12	10	0.11
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG13	10	0.11
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD11	7	0.11
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD12	7	0.11
(2,597)	1:2:A:GLU:HB2	1:9:A:ILE:HD13	7	0.11
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD11	5	0.11
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD12	5	0.11
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD13	5	0.11
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD11	8	0.11
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD12	8	0.11
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD13	8	0.11
(2,485)	1:11:A:TRP:HA	1:14:A:ASP:HB2	7	0.11
(2,455)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	6	0.11
(2,455)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	7	0.11
(2,281)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	3	0.11
(2,281)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	4	0.11
(2,281)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	5	0.11
(2,225)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	1	0.11
(2,221)	1:11:A:TRP:HD1	1:21:A:ARG:HD2	2	0.11
(2,201)	1:15:A:GLY:HA3	1:16:A:GLY:H	9	0.11
(2,177)	1:23:A:PRO:HB3	1:25:A:CYS:H	1	0.11
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG11	2	0.11
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG12	2	0.11
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG13	2	0.11
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG11	10	0.11
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG12	10	0.11
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG13	10	0.11
(1,554)	1:4:A:CYS:HA	1:7:A:LEU:HG	4	0.11
(1,524)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	4	0.11
(1,518)	1:1:A:GLU:HA	1:1:A:GLU:HB2	4	0.11
(1,518)	1:1:A:GLU:HA	1:1:A:GLU:HB2	8	0.11
(1,518)	1:1:A:GLU:HA	1:1:A:GLU:HB2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,506)	1:18:A:SER:HB2	1:19:A:SER:H	4	0.11
(1,489)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	5	0.11
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG2	1	0.11
(1,475)	1:11:A:TRP:HB2	1:24:A:PRO:HG3	1	0.11
(1,408)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	1	0.11
(1,408)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	4	0.11
(1,408)	1:22:A:PRO:HB2	1:22:A:PRO:HG2	8	0.11
(1,405)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	7	0.11
(1,392)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	5	0.11
(1,392)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	5	0.11
(1,380)	1:21:A:ARG:HA	1:21:A:ARG:HB2	3	0.11
(1,380)	1:21:A:ARG:HA	1:21:A:ARG:HB2	4	0.11
(1,374)	1:19:A:SER:HA	1:19:A:SER:HB2	7	0.11
(1,334)	1:12:A:LEU:HD11	1:12:A:LEU:HG	1	0.11
(1,334)	1:12:A:LEU:HD12	1:12:A:LEU:HG	1	0.11
(1,334)	1:12:A:LEU:HD13	1:12:A:LEU:HG	1	0.11
(1,329)	1:12:A:LEU:HA	1:12:A:LEU:HD11	8	0.11
(1,329)	1:12:A:LEU:HA	1:12:A:LEU:HD12	8	0.11
(1,329)	1:12:A:LEU:HA	1:12:A:LEU:HD13	8	0.11
(1,329)	1:12:A:LEU:HA	1:12:A:LEU:HD11	10	0.11
(1,329)	1:12:A:LEU:HA	1:12:A:LEU:HD12	10	0.11
(1,329)	1:12:A:LEU:HA	1:12:A:LEU:HD13	10	0.11
(1,312)	1:10:A:GLN:HA	1:10:A:GLN:HG2	4	0.11
(1,312)	1:10:A:GLN:HA	1:10:A:GLN:HG2	6	0.11
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	1	0.11
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	1	0.11
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	1	0.11
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	6	0.11
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	6	0.11
(1,311)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	6	0.11
(1,298)	1:9:A:ILE:HA	1:9:A:ILE:HG13	9	0.11
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB2	4	0.11
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB3	4	0.11
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB2	5	0.11
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB3	5	0.11
(1,262)	1:5:A:VAL:HA	1:5:A:VAL:HG21	4	0.11
(1,262)	1:5:A:VAL:HA	1:5:A:VAL:HG22	4	0.11
(1,262)	1:5:A:VAL:HA	1:5:A:VAL:HG23	4	0.11
(1,177)	1:23:A:PRO:HB3	1:25:A:CYS:H	6	0.11
(1,157)	1:8:A:TYR:HD1	1:23:A:PRO:HB2	6	0.11
(1,157)	1:8:A:TYR:HD2	1:23:A:PRO:HB2	6	0.11
(1,128)	1:8:A:TYR:HA	1:8:A:TYR:HD1	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:8:A:TYR:HA	1:8:A:TYR:HD2	4	0.11
(1,128)	1:8:A:TYR:HA	1:8:A:TYR:HD1	9	0.11
(1,128)	1:8:A:TYR:HA	1:8:A:TYR:HD2	9	0.11
(1,125)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	8	0.11
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	2	0.11
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	7	0.11
(1,91)	1:7:A:LEU:H	1:7:A:LEU:HB3	10	0.11
(1,65)	1:19:A:SER:H	1:19:A:SER:HB3	4	0.11
(1,65)	1:19:A:SER:H	1:19:A:SER:HB3	10	0.11
(1,61)	1:25:A:CYS:H	1:25:A:CYS:HB3	4	0.11
(1,42)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.11
(1,37)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	5	0.11
(1,17)	1:12:A:LEU:HB2	1:13:A:LYS:H	3	0.11
(3,501)	1:7:A:LEU:HB3	1:8:A:TYR:H	4	0.1
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD11	10	0.1
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD12	10	0.1
(3,470)	1:5:A:VAL:HA	1:9:A:ILE:HD13	10	0.1
(3,425)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	5	0.1
(3,257)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	8	0.1
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG11	1	0.1
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG12	1	0.1
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG13	1	0.1
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG11	3	0.1
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG12	3	0.1
(3,5)	1:5:A:VAL:H	1:5:A:VAL:HG13	3	0.1
(2,531)	1:7:A:LEU:HB3	1:8:A:TYR:H	4	0.1
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD11	10	0.1
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD12	10	0.1
(2,500)	1:5:A:VAL:HA	1:9:A:ILE:HD13	10	0.1
(2,455)	1:23:A:PRO:HB2	1:24:A:PRO:HD3	5	0.1
(2,281)	1:6:A:ARG:HB3	1:6:A:ARG:HG2	8	0.1
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG11	1	0.1
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG12	1	0.1
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG13	1	0.1
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG11	3	0.1
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG12	3	0.1
(2,6)	1:5:A:VAL:H	1:5:A:VAL:HG13	3	0.1
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG11	9	0.1
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG12	9	0.1
(1,594)	1:2:A:GLU:HB3	1:5:A:VAL:HG13	9	0.1
(1,568)	1:19:A:SER:HB3	1:21:A:ARG:HB3	4	0.1
(1,568)	1:19:A:SER:HB3	1:21:A:ARG:HB3	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:12:A:LEU:H	1:14:A:ASP:H	6	0.1
(1,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.1
(1,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	9	0.1
(1,545)	1:11:A:TRP:HE3	1:12:A:LEU:HG	10	0.1
(1,518)	1:1:A:GLU:HA	1:1:A:GLU:HB2	1	0.1
(1,518)	1:1:A:GLU:HA	1:1:A:GLU:HB2	7	0.1
(1,513)	1:23:A:PRO:HA	1:24:A:PRO:HD3	4	0.1
(1,511)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	9	0.1
(1,392)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	2	0.1
(1,392)	1:21:A:ARG:HB2	1:21:A:ARG:HG3	2	0.1
(1,384)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	6	0.1
(1,380)	1:21:A:ARG:HA	1:21:A:ARG:HB2	8	0.1
(1,374)	1:19:A:SER:HA	1:19:A:SER:HB2	3	0.1
(1,359)	1:17:A:PRO:HA	1:17:A:PRO:HG2	2	0.1
(1,359)	1:17:A:PRO:HA	1:17:A:PRO:HG3	2	0.1
(1,356)	1:17:A:PRO:HA	1:17:A:PRO:HD2	9	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB2	1	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB3	1	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB2	2	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB3	2	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB2	3	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB3	3	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB2	6	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB3	6	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB2	7	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB3	7	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB2	8	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB3	8	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB2	9	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB3	9	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB2	10	0.1
(1,296)	1:8:A:TYR:HA	1:8:A:TYR:HB3	10	0.1
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	7	0.1
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	7	0.1
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	7	0.1
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	7	0.1
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	7	0.1
(1,295)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	7	0.1
(1,248)	1:2:A:GLU:HA	1:2:A:GLU:HG2	5	0.1
(1,154)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	2	0.1
(1,130)	1:5:A:VAL:HA	1:8:A:TYR:HD1	4	0.1
(1,130)	1:5:A:VAL:HA	1:8:A:TYR:HD2	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:19:A:SER:H	1:19:A:SER:HB2	9	0.1
(1,37)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	6	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found