Full wwPDB NMR Structure Validation Report

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PDB ID	:	9G22
BMRB ID	:	34932
Title	:	Trp-cage fortified Tc5b-Exenatide chimera (Ex4-Tc5bDR) at 277K
Authors	:	Horvath, D.
Deposited on	:	2024-07-10

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 (i) 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 (1)) were used in the production of this report:

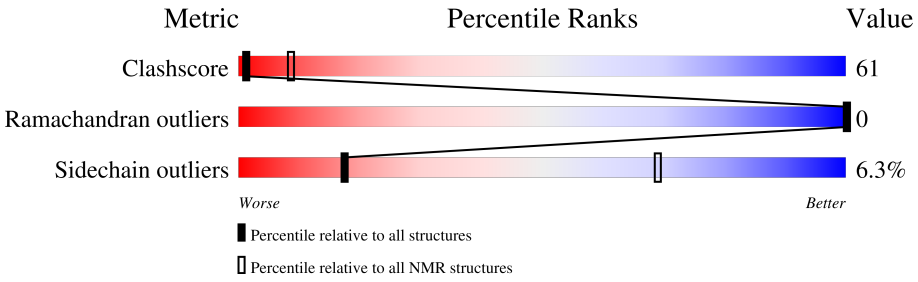
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 53%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	25	36% 48% · · 8%

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:24 (23)	0.11	4

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 385 atoms, of which 189 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Exendin-4.

Mol	Chain	Residues	Atoms					Trace
1	A	25	Total	C	H	N	O	0
			385	123	189	34	39	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	TYR	PHE	engineered mutation	UNP P26349
A	10	GLN	GLU	engineered mutation	UNP P26349
A	14	ASP	ASN	engineered mutation	UNP P26349
A	21	ARG	ALA	engineered mutation	UNP P26349

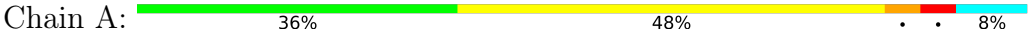
4 Residue-property plots (i)

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: Exendin-4

Chain A:



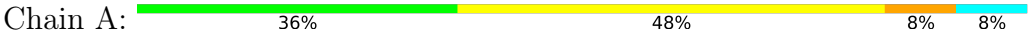
4.2 Scores per residue for each member of the ensemble

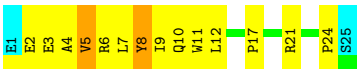
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Exendin-4

Chain A:





4.2.2 Score per residue for model 2

• Molecule 1: Exendin-4

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Exendin-4

Chain A:

4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Exendin-4

Chain A:

4.2.5 Score per residue for model 5

• Molecule 1: Exendin-4

Chain A:

4.2.6 Score per residue for model 6

• Molecule 1: Exendin-4

Chain A:

4.2.7 Score per residue for model 7

• Molecule 1: Exendin-4

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: Exendin-4

Chain A:

4.2.9 Score per residue for model 9

• Molecule 1: Exendin-4

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: Exendin-4

Chain A:

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	173
Number of shifts mapped to atoms	173
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	53%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.40±0.08	3±1/187 (1.4± 0.4%)	1.03±0.03	0±0/256 (0.0± 0.1%)
All	All	1.40	27/1870 (1.4%)	1.03	1/2560 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.7±0.5
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	8	TYR	CE1-CZ	8.57	1.49	1.38	7	7
1	A	8	TYR	CE2-CZ	-5.38	1.31	1.38	7	1
1	A	8	TYR	CB-CG	-5.33	1.43	1.51	9	10
1	A	8	TYR	CD1-CE1	-5.24	1.31	1.39	7	7
1	A	8	TYR	CD2-CE2	-5.06	1.31	1.39	1	2

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	21	ARG	N-CA-CB	-5.08	101.45	110.60	2	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	8	TYR	Sidechain	7

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	180	176	176	22±1
All	All	1800	1760	1760	216

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 61.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ILE:HA	1:A:12:LEU:HD12	0.87	1.46	1	10
1:A:8:TYR:CZ	1:A:12:LEU:HD11	0.78	2.13	7	10
1:A:8:TYR:O	1:A:11:TRP:HB3	0.75	1.81	4	10
1:A:3:GLU:O	1:A:6:ARG:HB2	0.74	1.83	3	10
1:A:3:GLU:HG3	1:A:7:LEU:CD1	0.72	2.15	4	1
1:A:3:GLU:HG3	1:A:7:LEU:HD13	0.70	1.63	4	1
1:A:8:TYR:CE1	1:A:12:LEU:HD11	0.69	2.22	3	10
1:A:4:ALA:HA	1:A:7:LEU:HD22	0.64	1.68	9	10
1:A:8:TYR:HE2	1:A:11:TRP:CZ3	0.63	2.12	6	10
1:A:3:GLU:HG2	1:A:7:LEU:CD1	0.62	2.24	2	9
1:A:3:GLU:O	1:A:7:LEU:HD13	0.61	1.94	9	10
1:A:2:GLU:O	1:A:5:VAL:HG13	0.57	1.99	8	9
1:A:7:LEU:O	1:A:10:GLN:HB3	0.56	2.00	3	10
1:A:11:TRP:CH2	1:A:17:PRO:HD3	0.55	2.37	1	10
1:A:11:TRP:CD1	1:A:21:ARG:HG2	0.55	2.37	2	10
1:A:8:TYR:CE2	1:A:11:TRP:CE3	0.53	2.97	9	10
1:A:3:GLU:HG2	1:A:7:LEU:HD13	0.53	1.80	5	9
1:A:8:TYR:HB2	1:A:24:PRO:HG2	0.50	1.84	10	9
1:A:8:TYR:CE2	1:A:11:TRP:CZ3	0.49	3.00	5	10
1:A:8:TYR:OH	1:A:12:LEU:HD11	0.49	2.08	5	6
1:A:5:VAL:HA	1:A:8:TYR:HB3	0.49	1.84	7	10
1:A:8:TYR:HA	1:A:24:PRO:CG	0.48	2.38	6	9
1:A:11:TRP:NE1	1:A:21:ARG:HG2	0.44	2.28	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:TYR:CD2	1:A:11:TRP:CE3	0.43	3.06	5	2
1:A:5:VAL:O	1:A:8:TYR:HB3	0.42	2.14	4	3
1:A:8:TYR:CE1	1:A:12:LEU:CD1	0.42	2.99	6	3
1:A:2:GLU:HB3	1:A:5:VAL:CG1	0.42	2.44	10	1
1:A:8:TYR:CA	1:A:24:PRO:HG2	0.42	2.44	9	4
1:A:2:GLU:O	1:A:6:ARG:HG2	0.41	2.16	4	1
1:A:11:TRP:CD2	1:A:16:GLY:HA2	0.40	2.51	7	1
1:A:7:LEU:O	1:A:11:TRP:N	0.40	2.54	4	1
1:A:8:TYR:HA	1:A:24:PRO:HG2	0.40	1.94	9	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	23/25 (92%)	22±1 (98±3%)	0±1 (2±3%)	0±0 (0±0%)	100	100
All	All	230/250 (92%)	225 (98%)	5 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	19/21 (90%)	18±0 (94±2%)	1±0 (6±2%)	17	69
All	All	190/210 (90%)	178 (94%)	12 (6%)	17	69

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	5	VAL	10
1	A	21	ARG	1
1	A	2	GLU	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 53% for the well-defined parts and 52% 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	173
Number of shifts mapped to atoms	173
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 53%, i.e. 163 atoms were assigned a chemical shift out of a possible 309. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	44/110 (40%)	44/45 (98%)	0/46 (0%)	0/19 (0%)
Sidechain	109/178 (61%)	109/115 (95%)	0/55 (0%)	0/8 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	163/309 (53%)	163/170 (96%)	0/111 (0%)	0/28 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 172 atoms were assigned a chemical shift out of a possible 329. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	47/120 (39%)	47/49 (96%)	0/50 (0%)	0/21 (0%)
Sidechain	115/188 (61%)	115/121 (95%)	0/59 (0%)	0/8 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	172/329 (52%)	172/180 (96%)	0/119 (0%)	0/30 (0%)

7.1.4 Statistically unusual chemical shifts (i)

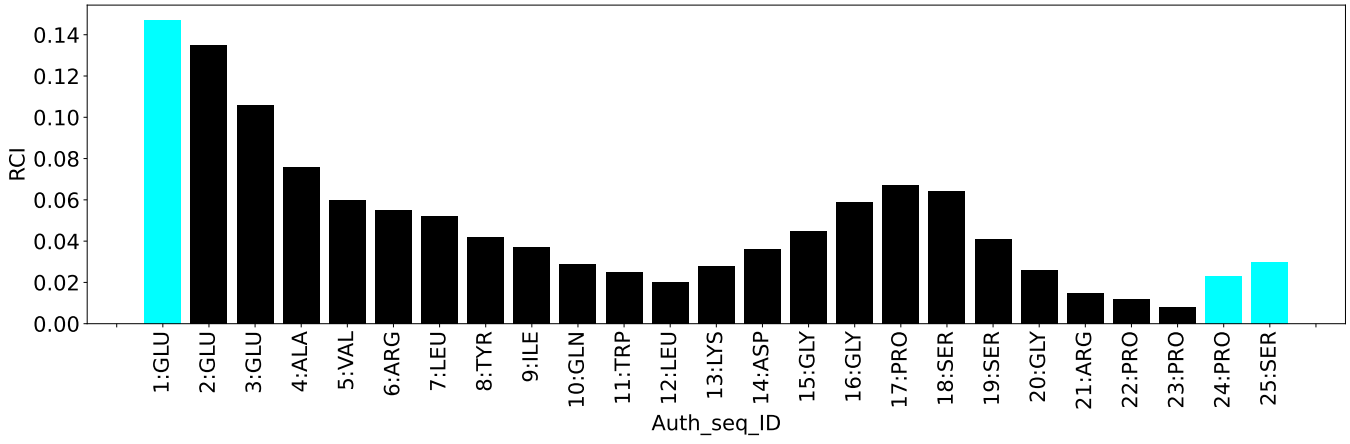
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	16	GLY	HA2	0.57	2.15 – 5.77	-9.3
1	A	23	PRO	HA	2.40	2.78 – 6.00	-6.2
1	A	23	PRO	HB2	0.22	0.37 – 3.78	-5.4

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	1580
Intra-residue (|i-j|=0)	690
Sequential (|i-j|=1)	334
Medium range (|i-j|>1 and |i-j|<5)	344
Long range (|i-j|≥5)	212
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	63.2
Number of long range restraints per residue[1]	8.5

[1]Long 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)	68.2	0.2
0.2-0.5 (Medium)	111.6	0.5
>0.5 (Large)	111.0	4.42

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 (i)

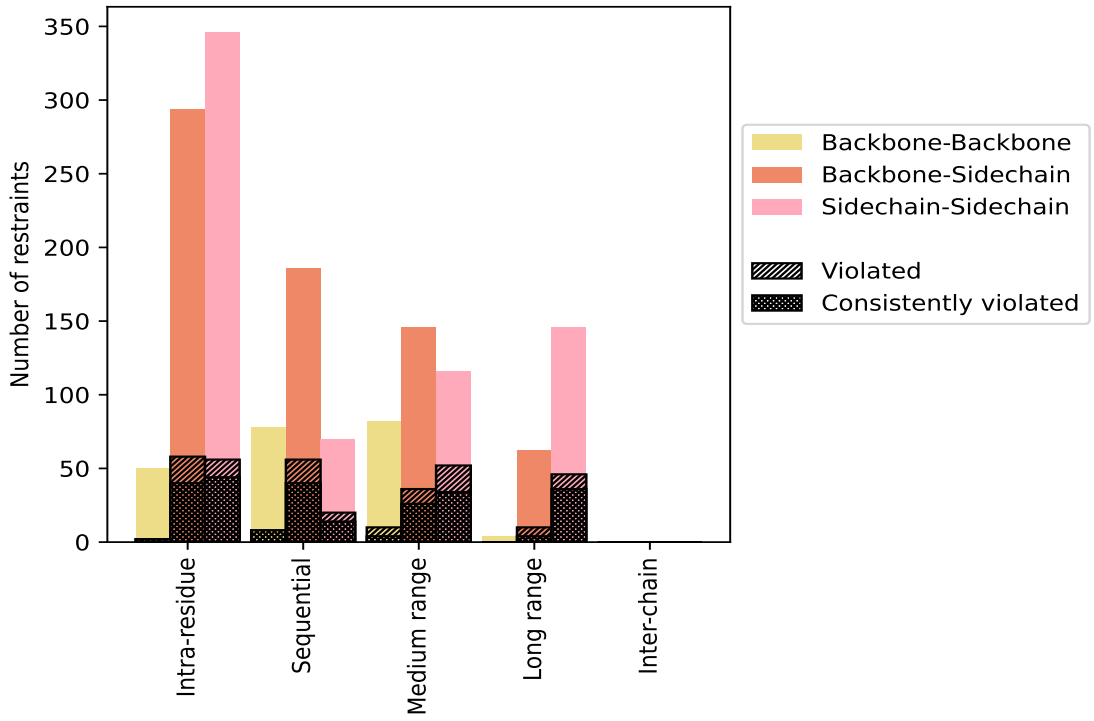
9.1 Summary of distance violations (i)

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)	690	43.7	116	16.8	7.3	86	12.5	5.4
Backbone-Backbone	50	3.2	2	4.0	0.1	2	4.0	0.1
Backbone-Sidechain	294	18.6	58	19.7	3.7	40	13.6	2.5
Sidechain-Sidechain	346	21.9	56	16.2	3.5	44	12.7	2.8
Sequential (|i-j|=1)	334	21.1	84	25.1	5.3	62	18.6	3.9
Backbone-Backbone	78	4.9	8	10.3	0.5	8	10.3	0.5
Backbone-Sidechain	186	11.8	56	30.1	3.5	40	21.5	2.5
Sidechain-Sidechain	70	4.4	20	28.6	1.3	14	20.0	0.9
Medium range (|i-j|>1 & |i-j|<5)	344	21.8	98	28.5	6.2	64	18.6	4.1
Backbone-Backbone	82	5.2	10	12.2	0.6	4	4.9	0.3
Backbone-Sidechain	146	9.2	36	24.7	2.3	26	17.8	1.6
Sidechain-Sidechain	116	7.3	52	44.8	3.3	34	29.3	2.2
Long range (|i-j|≥5)	212	13.4	56	26.4	3.5	40	18.9	2.5
Backbone-Backbone	4	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	62	3.9	10	16.1	0.6	4	6.5	0.3
Sidechain-Sidechain	146	9.2	46	31.5	2.9	36	24.7	2.3
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1580	100.0	354	22.4	22.4	252	15.9	15.9
Backbone-Backbone	214	13.5	20	9.3	1.3	14	6.5	0.9
Backbone-Sidechain	688	43.5	160	23.3	10.1	110	16.0	7.0
Sidechain-Sidechain	678	42.9	174	25.7	11.0	128	18.9	8.1

[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



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

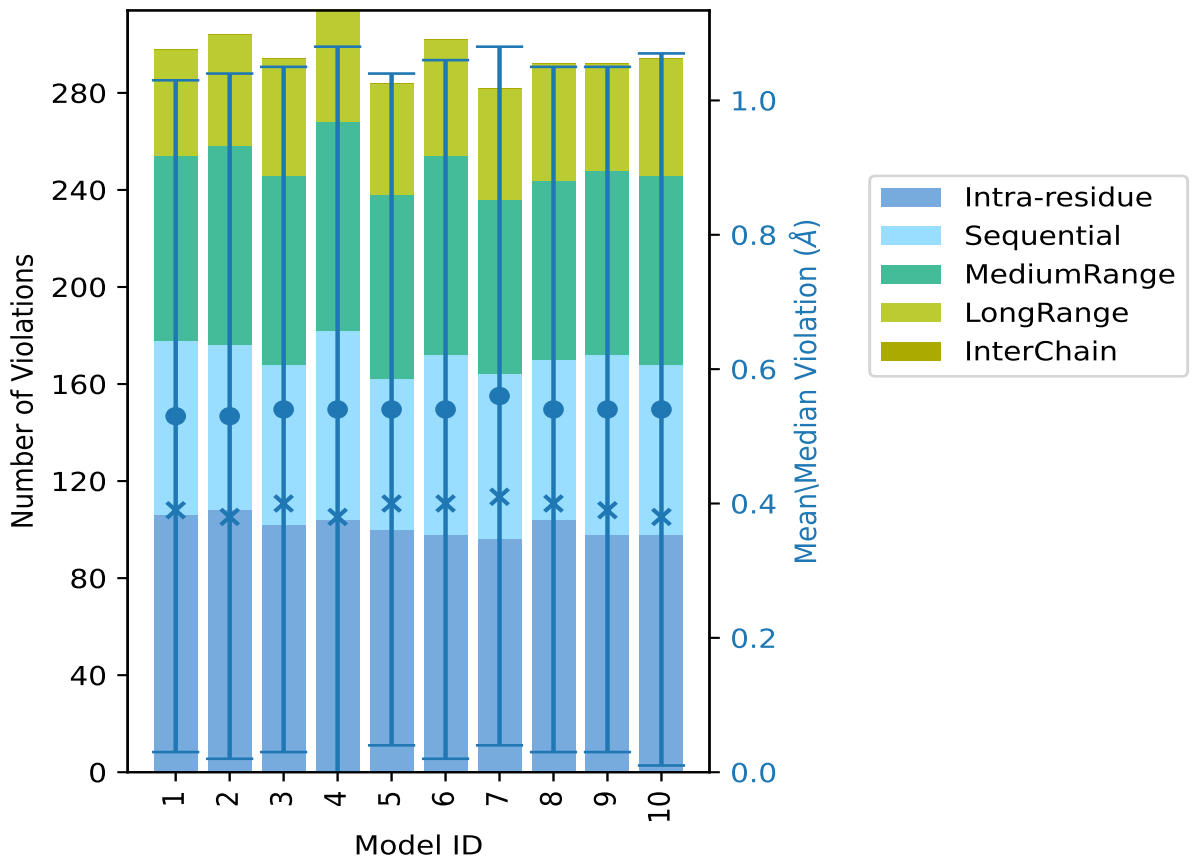
9.2 Distance violation statistics for each model

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	106	72	76	44	0	298	0.53	4.18	0.5	0.39
2	108	68	82	46	0	304	0.53	4.28	0.51	0.38
3	102	66	78	48	0	294	0.54	4.32	0.51	0.4
4	104	78	86	46	0	314	0.54	4.34	0.54	0.38
5	100	62	76	46	0	284	0.54	4.03	0.5	0.4
6	98	74	82	48	0	302	0.54	4.34	0.52	0.4
7	96	68	72	46	0	282	0.56	4.37	0.52	0.41
8	104	66	74	48	0	292	0.54	4.32	0.51	0.4
9	98	74	76	44	0	292	0.54	4.25	0.51	0.39
10	98	70	78	48	0	294	0.54	4.42	0.53	0.38

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

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, 1226(IR:574, SQ:250, MR:246, LR:156, 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]	%
8	4	14	0	0	26	1	10.0
0	6	0	6	0	12	2	20.0
2	4	2	4	0	12	3	30.0

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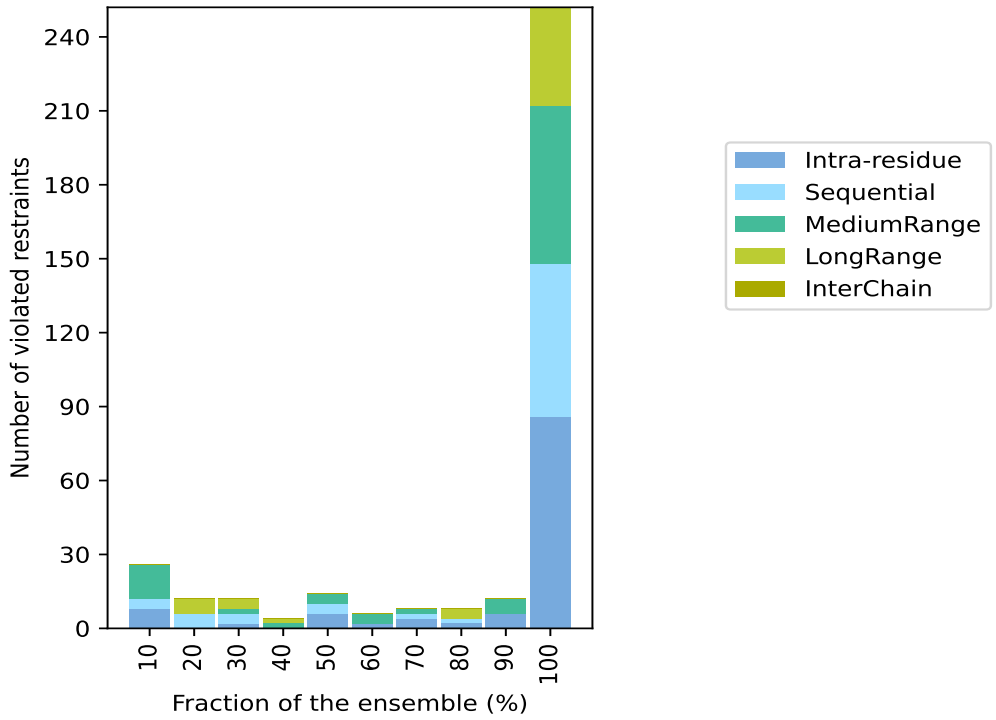
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	2	2	0	4	4	40.0
6	4	4	0	0	14	5	50.0
2	0	4	0	0	6	6	60.0
4	2	2	0	0	8	7	70.0
2	2	0	4	0	8	8	80.0
6	0	6	0	0	12	9	90.0
86	62	64	40	0	252	10	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble

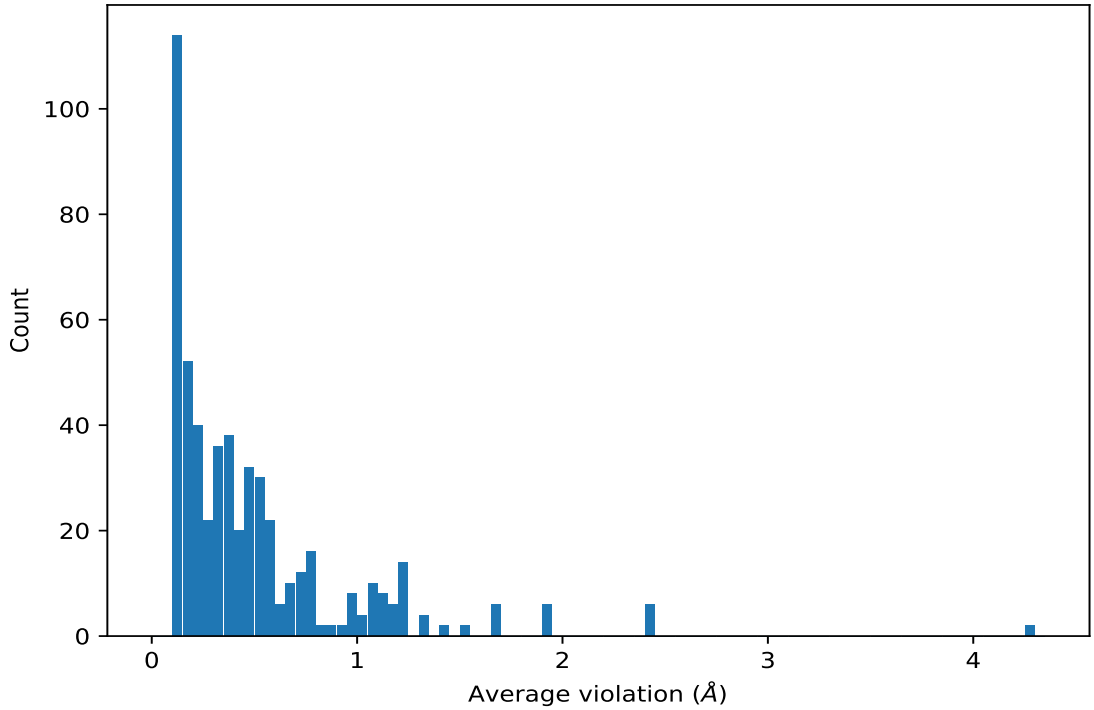


9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,311)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	10	4.29	0.11	4.32
(3,29)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	10	4.29	0.11	4.32
(1,787)	1:5:A:VAL:HG11	1:9:A:ILE:HB	10	2.43	0.04	2.45
(1,787)	1:5:A:VAL:HG12	1:9:A:ILE:HB	10	2.43	0.04	2.45
(1,787)	1:5:A:VAL:HG13	1:9:A:ILE:HB	10	2.43	0.04	2.45
(3,84)	1:5:A:VAL:HG11	1:9:A:ILE:HB	10	2.43	0.04	2.45
(3,84)	1:5:A:VAL:HG12	1:9:A:ILE:HB	10	2.43	0.04	2.45
(3,84)	1:5:A:VAL:HG13	1:9:A:ILE:HB	10	2.43	0.04	2.45
(1,725)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	10	1.94	0.04	1.93
(1,725)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	10	1.94	0.04	1.93
(1,725)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	10	1.94	0.04	1.93
(3,77)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	10	1.94	0.04	1.93
(3,77)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	10	1.94	0.04	1.93
(3,77)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	10	1.94	0.04	1.93
(1,495)	1:3:A:GLU:HB3	1:7:A:LEU:H	10	1.68	0.12	1.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,58)	1:3:A:GLU:HB3	1:7:A:LEU:H	10	1.68	0.12	1.65
(1,459)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	10	1.66	0.04	1.66
(1,459)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	10	1.66	0.04	1.66
(3,49)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	10	1.66	0.04	1.66
(3,49)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	10	1.66	0.04	1.66
(1,763)	1:14:A:ASP:HB2	1:19:A:SER:HA	10	1.53	0.03	1.52
(2,683)	1:14:A:ASP:HB2	1:19:A:SER:HA	10	1.53	0.03	1.52
(1,778)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	10	1.43	0.4	1.3
(2,697)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	10	1.43	0.4	1.3
(1,411)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	10	1.32	0.05	1.32
(2,368)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	10	1.32	0.05	1.32
(1,560)	1:5:A:VAL:HB	1:6:A:ARG:H	10	1.3	0.03	1.31
(3,68)	1:5:A:VAL:HB	1:6:A:ARG:H	10	1.3	0.03	1.31
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	10	1.22	0.06	1.25
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	10	1.22	0.06	1.25
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	10	1.22	0.06	1.25
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	10	1.22	0.06	1.25
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	10	1.22	0.06	1.25
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	10	1.22	0.06	1.25
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	10	1.22	0.06	1.25
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	10	1.22	0.06	1.25
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	10	1.22	0.06	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	10	1.22	0.06	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	10	1.22	0.06	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	10	1.22	0.06	1.25
(1,640)	1:3:A:GLU:HA	1:7:A:LEU:HG	10	1.2	0.11	1.21
(3,73)	1:3:A:GLU:HA	1:7:A:LEU:HG	10	1.2	0.11	1.21
(1,423)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.16	0.01	1.16
(3,44)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.16	0.01	1.16
(1,417)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	1.15	0.02	1.15
(2,374)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	1.15	0.02	1.15
(1,499)	1:4:A:ALA:H	1:7:A:LEU:HB3	10	1.15	0.02	1.15
(3,60)	1:4:A:ALA:H	1:7:A:LEU:HB3	10	1.15	0.02	1.15
(1,504)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	1.11	0.02	1.12
(1,504)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	1.11	0.02	1.12
(1,504)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	1.11	0.02	1.12
(3,61)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	1.11	0.02	1.12
(3,61)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	1.11	0.02	1.12
(3,61)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	1.11	0.02	1.12
(1,378)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	10	1.1	0.09	1.11
(2,338)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	10	1.1	0.09	1.11
(1,461)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	10	1.09	0.03	1.08

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,461)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	10	1.09	0.03	1.08
(3,51)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	10	1.09	0.03	1.08
(3,51)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	10	1.09	0.03	1.08
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	10	1.08	0.05	1.07
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	10	1.08	0.05	1.07
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	10	1.08	0.05	1.07
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	10	1.08	0.05	1.07
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	10	1.08	0.05	1.07
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	10	1.08	0.05	1.07
(1,383)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	10	1.03	0.06	1.06
(2,342)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	10	1.03	0.06	1.06
(1,777)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	10	1.02	0.05	1.04
(2,696)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	10	1.02	0.05	1.04
(1,577)	1:23:A:PRO:HB3	1:25:A:SER:H	10	0.98	0.49	1.1
(2,507)	1:23:A:PRO:HB3	1:25:A:SER:H	10	0.98	0.49	1.1
(1,657)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.97	0.02	0.96
(2,584)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.97	0.02	0.96
(1,776)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	10	0.96	0.04	0.96
(2,695)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	10	0.96	0.04	0.96
(1,81)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.96	0.02	0.96
(3,13)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.96	0.02	0.96
(1,15)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.94	0.06	0.94
(3,3)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.94	0.06	0.94
(1,382)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.87	0.01	0.86
(3,41)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.87	0.01	0.86
(1,240)	1:21:A:ARG:H	1:21:A:ARG:HG3	10	0.78	0.06	0.8
(2,214)	1:21:A:ARG:H	1:21:A:ARG:HG3	10	0.78	0.06	0.8
(1,532)	1:21:A:ARG:H	1:22:A:PRO:HD2	10	0.77	0.09	0.77
(3,64)	1:21:A:ARG:H	1:22:A:PRO:HD2	10	0.77	0.09	0.77
(1,434)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.77	0.03	0.78
(2,390)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.77	0.03	0.78
(1,460)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.77	0.0	0.77
(3,50)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.77	0.0	0.77
(1,494)	1:3:A:GLU:HB2	1:7:A:LEU:H	10	0.75	0.05	0.76
(3,57)	1:3:A:GLU:HB2	1:7:A:LEU:H	10	0.75	0.05	0.76
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.73	0.01	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.73	0.01	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.73	0.01	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.73	0.01	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.73	0.01	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.73	0.01	0.72
(1,386)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	10	0.71	0.1	0.75

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,42)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	10	0.71	0.1	0.75
(1,355)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.7	0.07	0.72
(1,355)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.7	0.07	0.72
(2,318)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.7	0.07	0.72
(2,318)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.7	0.07	0.72
(1,55)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.67	0.02	0.68
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.67	0.02	0.68
(1,599)	1:3:A:GLU:HG2	1:5:A:VAL:H	10	0.66	0.36	0.46
(3,72)	1:3:A:GLU:HG2	1:5:A:VAL:H	10	0.66	0.36	0.46
(1,733)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	10	0.65	0.1	0.63
(1,733)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	10	0.65	0.1	0.63
(1,733)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	10	0.65	0.1	0.63
(2,655)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	10	0.65	0.1	0.63
(2,655)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	10	0.65	0.1	0.63
(2,655)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	10	0.65	0.1	0.63
(1,128)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.62	0.03	0.62
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.62	0.03	0.62
(1,257)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	10	0.62	0.01	0.62
(2,231)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	10	0.62	0.01	0.62
(1,781)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.6	0.0	0.6
(3,82)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.6	0.0	0.6
(1,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.58	0.2	0.48
(3,4)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.58	0.2	0.48
(1,410)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.58	0.03	0.57
(2,367)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.58	0.03	0.57
(1,365)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	10	0.58	0.02	0.57
(2,325)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	10	0.58	0.02	0.57
(1,406)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	10	0.56	0.02	0.57
(2,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	10	0.56	0.02	0.57
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.55	0.01	0.56
(2,92)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.55	0.01	0.56
(1,260)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.55	0.01	0.55
(2,233)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.55	0.01	0.55
(1,353)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	10	0.55	0.1	0.55
(1,353)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	10	0.55	0.1	0.55
(3,37)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	10	0.55	0.1	0.55
(3,37)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	10	0.55	0.1	0.55
(1,30)	1:5:A:VAL:H	1:5:A:VAL:HB	10	0.55	0.08	0.52
(3,6)	1:5:A:VAL:H	1:5:A:VAL:HB	10	0.55	0.08	0.52
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.55	0.02	0.56
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.55	0.02	0.56
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.55	0.02	0.56

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.55	0.02	0.56
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD2	10	0.54	0.02	0.55
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD3	10	0.54	0.02	0.55
(1,389)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	10	0.54	0.01	0.54
(2,347)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	10	0.54	0.01	0.54
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD2	10	0.54	0.02	0.55
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD3	10	0.54	0.02	0.55
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.54	0.01	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.54	0.01	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.54	0.01	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.54	0.01	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.54	0.01	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.54	0.01	0.54
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	10	0.53	0.1	0.56
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	10	0.53	0.1	0.56
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	10	0.53	0.1	0.56
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	10	0.53	0.1	0.56
(1,579)	1:24:A:PRO:HB3	1:25:A:SER:H	10	0.52	0.06	0.5
(3,71)	1:24:A:PRO:HB3	1:25:A:SER:H	10	0.52	0.06	0.5
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	0.51	0.17	0.42
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	0.51	0.17	0.42
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	0.51	0.17	0.42
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	0.51	0.17	0.42
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	0.51	0.17	0.42
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	0.51	0.17	0.42
(1,522)	1:7:A:LEU:HG	1:8:A:TYR:H	10	0.51	0.04	0.5
(3,63)	1:7:A:LEU:HG	1:8:A:TYR:H	10	0.51	0.04	0.5
(1,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	10	0.51	0.13	0.55
(3,1)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	10	0.51	0.13	0.55
(1,667)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	10	0.5	0.07	0.5
(3,74)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	10	0.5	0.07	0.5
(1,601)	1:5:A:VAL:H	1:6:A:ARG:HB3	10	0.49	0.11	0.46
(2,529)	1:5:A:VAL:H	1:6:A:ARG:HB3	10	0.49	0.11	0.46
(1,124)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	10	0.49	0.0	0.49
(3,18)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	10	0.49	0.0	0.49
(1,576)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.49	0.03	0.48
(1,576)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.49	0.03	0.48
(1,576)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.49	0.03	0.48
(3,70)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.49	0.03	0.48
(3,70)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.49	0.03	0.48
(3,70)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.49	0.03	0.48
(1,278)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	10	0.48	0.14	0.49

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,250)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	10	0.48	0.14	0.49
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:H	10	0.45	0.01	0.45
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:H	10	0.45	0.01	0.45
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:H	10	0.45	0.01	0.45
(3,62)	1:12:A:LEU:HD21	1:13:A:LYS:H	10	0.45	0.01	0.45
(3,62)	1:12:A:LEU:HD22	1:13:A:LYS:H	10	0.45	0.01	0.45
(3,62)	1:12:A:LEU:HD23	1:13:A:LYS:H	10	0.45	0.01	0.45
(1,350)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	0.45	0.07	0.41
(1,350)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	0.45	0.07	0.41
(3,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	0.45	0.07	0.41
(3,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	0.45	0.07	0.41
(1,320)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	10	0.45	0.06	0.46
(1,320)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	10	0.45	0.06	0.46
(3,30)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	10	0.45	0.06	0.46
(3,30)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	10	0.45	0.06	0.46
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.45	0.0	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.45	0.0	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.45	0.0	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.45	0.0	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.45	0.0	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.45	0.0	0.45
(1,337)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	0.42	0.04	0.44
(1,337)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	0.42	0.04	0.44
(3,33)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	0.42	0.04	0.44
(3,33)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	0.42	0.04	0.44
(1,571)	1:7:A:LEU:HB3	1:10:A:GLN:H	10	0.42	0.01	0.42
(3,69)	1:7:A:LEU:HB3	1:10:A:GLN:H	10	0.42	0.01	0.42
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	10	0.41	0.07	0.4
(2,160)	1:13:A:LYS:H	1:13:A:LYS:HG2	10	0.41	0.07	0.4
(1,342)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	10	0.4	0.0	0.4
(3,35)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	10	0.4	0.0	0.4
(1,247)	1:21:A:ARG:HA	1:21:A:ARG:HG2	10	0.4	0.02	0.41
(2,221)	1:21:A:ARG:HA	1:21:A:ARG:HG2	10	0.4	0.02	0.41
(1,457)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	10	0.4	0.03	0.41
(1,457)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	10	0.4	0.03	0.41
(3,48)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	10	0.4	0.03	0.41
(3,48)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	10	0.4	0.03	0.41
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.39	0.03	0.4
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.39	0.03	0.4
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.39	0.03	0.4
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.39	0.03	0.4
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.39	0.03	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.39	0.03	0.4
(1,330)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	10	0.39	0.04	0.4
(1,330)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	10	0.39	0.04	0.4
(3,31)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	10	0.39	0.04	0.4
(3,31)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	10	0.39	0.04	0.4
(1,396)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.39	0.01	0.39
(3,43)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.39	0.01	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG11	10	0.38	0.02	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG12	10	0.38	0.02	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG13	10	0.38	0.02	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG11	10	0.38	0.02	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG12	10	0.38	0.02	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG13	10	0.38	0.02	0.39
(1,498)	1:4:A:ALA:HB1	1:7:A:LEU:H	10	0.37	0.02	0.38
(1,498)	1:4:A:ALA:HB2	1:7:A:LEU:H	10	0.37	0.02	0.38
(1,498)	1:4:A:ALA:HB3	1:7:A:LEU:H	10	0.37	0.02	0.38
(3,59)	1:4:A:ALA:HB1	1:7:A:LEU:H	10	0.37	0.02	0.38
(3,59)	1:4:A:ALA:HB2	1:7:A:LEU:H	10	0.37	0.02	0.38
(3,59)	1:4:A:ALA:HB3	1:7:A:LEU:H	10	0.37	0.02	0.38
(1,747)	1:17:A:PRO:HA	1:19:A:SER:H	10	0.36	0.01	0.36
(3,80)	1:17:A:PRO:HA	1:19:A:SER:H	10	0.36	0.01	0.36
(1,239)	1:21:A:ARG:H	1:21:A:ARG:HG2	10	0.36	0.05	0.36
(3,26)	1:21:A:ARG:H	1:21:A:ARG:HG2	10	0.36	0.05	0.36
(1,443)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.36	0.01	0.36
(3,46)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.36	0.01	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	10	0.36	0.01	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	10	0.36	0.01	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	10	0.36	0.01	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	10	0.36	0.01	0.36
(1,526)	1:17:A:PRO:HB3	1:19:A:SER:H	10	0.36	0.02	0.36
(2,463)	1:17:A:PRO:HB3	1:19:A:SER:H	10	0.36	0.02	0.36
(1,127)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.35	0.01	0.35
(3,19)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.35	0.01	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.34	0.01	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.34	0.01	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.34	0.01	0.34
(1,717)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	10	0.34	0.02	0.34
(1,717)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	10	0.34	0.02	0.34
(1,717)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	10	0.34	0.02	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.34	0.01	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.34	0.01	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.34	0.01	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,76)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	10	0.34	0.02	0.34
(3,76)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	10	0.34	0.02	0.34
(3,76)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	10	0.34	0.02	0.34
(1,71)	1:7:A:LEU:HB2	1:7:A:LEU:HG	10	0.34	0.0	0.34
(3,11)	1:7:A:LEU:HB2	1:7:A:LEU:HG	10	0.34	0.0	0.34
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD11	10	0.32	0.02	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD12	10	0.32	0.02	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD13	10	0.32	0.02	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD11	10	0.32	0.02	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD12	10	0.32	0.02	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD13	10	0.32	0.02	0.32
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.32	0.01	0.32
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.32	0.01	0.32
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.32	0.01	0.32
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.32	0.01	0.32
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.32	0.01	0.32
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.32	0.01	0.32
(1,478)	1:16:A:GLY:H	1:17:A:PRO:HD2	10	0.31	0.01	0.32
(3,54)	1:16:A:GLY:H	1:17:A:PRO:HD2	10	0.31	0.01	0.32
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	10	0.3	0.02	0.3
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	10	0.3	0.02	0.3
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	10	0.3	0.02	0.3
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	10	0.3	0.02	0.3
(1,481)	1:16:A:GLY:H	1:17:A:PRO:HD3	10	0.3	0.01	0.3
(3,55)	1:16:A:GLY:H	1:17:A:PRO:HD3	10	0.3	0.01	0.3
(1,209)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	10	0.3	0.01	0.3
(2,185)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	10	0.3	0.01	0.3
(1,786)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	0.28	0.01	0.28
(1,786)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	0.28	0.01	0.28
(1,786)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	0.28	0.01	0.28
(3,83)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	0.28	0.01	0.28
(3,83)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	0.28	0.01	0.28
(3,83)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	0.28	0.01	0.28
(1,552)	1:14:A:ASP:H	1:15:A:GLY:HA3	10	0.28	0.01	0.28
(3,66)	1:14:A:ASP:H	1:15:A:GLY:HA3	10	0.28	0.01	0.28
(1,581)	1:17:A:PRO:HB3	1:18:A:SER:H	10	0.27	0.05	0.27
(2,510)	1:17:A:PRO:HB3	1:18:A:SER:H	10	0.27	0.05	0.27
(1,216)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.26	0.0	0.26
(3,25)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.26	0.0	0.26
(1,681)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	10	0.26	0.06	0.25
(2,607)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	10	0.26	0.06	0.25
(1,352)	1:8:A:TYR:HD1	1:9:A:ILE:HB	10	0.26	0.04	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,352)	1:8:A:TYR:HD2	1:9:A:ILE:HB	10	0.26	0.04	0.28
(2,316)	1:8:A:TYR:HD1	1:9:A:ILE:HB	10	0.26	0.04	0.28
(2,316)	1:8:A:TYR:HD2	1:9:A:ILE:HB	10	0.26	0.04	0.28
(1,405)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	10	0.25	0.03	0.26
(2,362)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	10	0.25	0.03	0.26
(1,165)	1:10:A:GLN:HA	1:13:A:LYS:H	10	0.25	0.01	0.25
(3,22)	1:10:A:GLN:HA	1:13:A:LYS:H	10	0.25	0.01	0.25
(1,728)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.24	0.02	0.25
(1,728)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.24	0.02	0.25
(1,728)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.24	0.02	0.25
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.24	0.02	0.25
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.24	0.02	0.25
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.24	0.02	0.25
(1,689)	1:3:A:GLU:HG2	1:7:A:LEU:HG	10	0.23	0.27	0.15
(2,615)	1:3:A:GLU:HG2	1:7:A:LEU:HG	10	0.23	0.27	0.15
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.23	0.0	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.23	0.0	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.23	0.0	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.23	0.0	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.23	0.0	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.23	0.0	0.23
(1,402)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	10	0.22	0.03	0.24
(2,359)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	10	0.22	0.03	0.24
(1,274)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.22	0.1	0.22
(3,28)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.22	0.1	0.22
(1,493)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.22	0.01	0.22
(3,56)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.22	0.01	0.22
(1,435)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.21	0.04	0.22
(2,391)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.21	0.04	0.22
(1,548)	1:5:A:VAL:HA	1:6:A:ARG:H	10	0.21	0.01	0.21
(3,65)	1:5:A:VAL:HA	1:6:A:ARG:H	10	0.21	0.01	0.21
(1,673)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.21	0.01	0.21
(2,599)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.21	0.01	0.21
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.21	0.03	0.2
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.21	0.03	0.2
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.21	0.03	0.2
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.21	0.03	0.2
(1,161)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.2	0.01	0.2
(3,21)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.2	0.01	0.2
(1,742)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	10	0.19	0.02	0.19
(1,742)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	10	0.19	0.02	0.19
(3,79)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	10	0.19	0.02	0.19

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,79)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	10	0.19	0.02	0.19
(1,426)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	10	0.19	0.0	0.19
(2,382)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	10	0.19	0.0	0.19
(1,185)	1:13:A:LYS:HA	1:14:A:ASP:H	10	0.19	0.01	0.19
(3,24)	1:13:A:LYS:HA	1:14:A:ASP:H	10	0.19	0.01	0.19
(1,744)	1:6:A:ARG:HB3	1:7:A:LEU:H	10	0.18	0.01	0.18
(2,665)	1:6:A:ARG:HB3	1:7:A:LEU:H	10	0.18	0.01	0.18
(1,569)	1:13:A:LYS:HG2	1:14:A:ASP:H	10	0.17	0.01	0.17
(2,501)	1:13:A:LYS:HG2	1:14:A:ASP:H	10	0.17	0.01	0.17
(1,559)	1:10:A:GLN:HB2	1:11:A:TRP:H	10	0.17	0.02	0.16
(3,67)	1:10:A:GLN:HB2	1:11:A:TRP:H	10	0.17	0.02	0.16
(1,630)	1:22:A:PRO:HA	1:23:A:PRO:HG2	10	0.16	0.03	0.19
(2,558)	1:22:A:PRO:HA	1:23:A:PRO:HG2	10	0.16	0.03	0.19
(1,231)	1:20:A:GLY:H	1:20:A:GLY:HA3	10	0.15	0.01	0.15
(2,206)	1:20:A:GLY:H	1:20:A:GLY:HA3	10	0.15	0.01	0.15
(1,669)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	10	0.15	0.02	0.15
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	10	0.15	0.02	0.15
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	10	0.15	0.02	0.15
(2,595)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	10	0.15	0.02	0.15
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	10	0.15	0.02	0.15
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	10	0.15	0.02	0.15
(1,537)	1:7:A:LEU:HA	1:8:A:TYR:H	10	0.15	0.01	0.15
(2,473)	1:7:A:LEU:HA	1:8:A:TYR:H	10	0.15	0.01	0.15
(1,566)	1:13:A:LYS:HD2	1:14:A:ASP:H	10	0.14	0.02	0.13
(1,566)	1:13:A:LYS:HD3	1:14:A:ASP:H	10	0.14	0.02	0.13
(2,498)	1:13:A:LYS:HD2	1:14:A:ASP:H	10	0.14	0.02	0.13
(2,498)	1:13:A:LYS:HD3	1:14:A:ASP:H	10	0.14	0.02	0.13
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD11	10	0.14	0.01	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD12	10	0.14	0.01	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD13	10	0.14	0.01	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD11	10	0.14	0.01	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD12	10	0.14	0.01	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD13	10	0.14	0.01	0.14
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	10	0.12	0.0	0.12
(2,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	10	0.12	0.0	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD11	10	0.12	0.01	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD12	10	0.12	0.01	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD13	10	0.12	0.01	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD11	10	0.12	0.01	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD12	10	0.12	0.01	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD13	10	0.12	0.01	0.12
(1,463)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	10	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,412)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	10	0.12	0.0	0.12
(1,14)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	9	0.4	0.01	0.4
(3,2)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	9	0.4	0.01	0.4
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	9	0.18	0.04	0.19
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	9	0.18	0.04	0.19
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	9	0.18	0.04	0.19
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	9	0.18	0.04	0.19
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	9	0.18	0.04	0.19
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	9	0.18	0.04	0.19
(1,466)	1:2:A:GLU:HA	1:2:A:GLU:HB3	9	0.17	0.02	0.17
(2,414)	1:2:A:GLU:HA	1:2:A:GLU:HB3	9	0.17	0.02	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	9	0.16	0.03	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	9	0.16	0.03	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	9	0.16	0.03	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	9	0.16	0.03	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	9	0.16	0.03	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	9	0.16	0.03	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	9	0.16	0.03	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	9	0.16	0.03	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	9	0.16	0.03	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	9	0.16	0.03	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	9	0.16	0.03	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	9	0.16	0.03	0.17
(1,475)	1:4:A:ALA:HA	1:7:A:LEU:H	9	0.14	0.02	0.14
(3,53)	1:4:A:ALA:HA	1:7:A:LEU:H	9	0.14	0.02	0.14
(1,39)	1:6:A:ARG:HA	1:6:A:ARG:HG3	9	0.13	0.01	0.13
(2,32)	1:6:A:ARG:HA	1:6:A:ARG:HG3	9	0.13	0.01	0.13
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE1	8	0.15	0.02	0.16
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE2	8	0.15	0.02	0.16
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE1	8	0.15	0.02	0.16
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE2	8	0.15	0.02	0.16
(1,360)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	8	0.13	0.01	0.13
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	8	0.13	0.01	0.13
(1,385)	1:11:A:TRP:HD1	1:23:A:PRO:HA	8	0.12	0.02	0.11
(2,344)	1:11:A:TRP:HD1	1:23:A:PRO:HA	8	0.12	0.02	0.11
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	8	0.12	0.01	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	8	0.12	0.01	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	8	0.12	0.01	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	8	0.12	0.01	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	8	0.12	0.01	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	8	0.12	0.01	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	8	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	8	0.12	0.01	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	8	0.12	0.01	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	8	0.12	0.01	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	8	0.12	0.01	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	8	0.12	0.01	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	8	0.12	0.01	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	8	0.12	0.01	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	8	0.12	0.01	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	8	0.12	0.01	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	8	0.12	0.01	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	8	0.12	0.01	0.12
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	7	0.75	0.32	0.91
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	7	0.75	0.32	0.91
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	7	0.75	0.32	0.91
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	7	0.75	0.32	0.91
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	7	0.75	0.32	0.91
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	7	0.75	0.32	0.91
(1,227)	1:18:A:SER:H	1:18:A:SER:HB3	7	0.21	0.0	0.21
(2,202)	1:18:A:SER:H	1:18:A:SER:HB3	7	0.21	0.0	0.21
(1,534)	1:18:A:SER:HB3	1:19:A:SER:H	7	0.2	0.01	0.21
(2,470)	1:18:A:SER:HB3	1:19:A:SER:H	7	0.2	0.01	0.21
(1,208)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	7	0.11	0.01	0.11
(2,184)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	7	0.11	0.01	0.11
(1,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	6	0.42	0.01	0.42
(2,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	6	0.42	0.01	0.42
(1,692)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	6	0.12	0.01	0.12
(2,618)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	6	0.12	0.01	0.12
(1,376)	1:8:A:TYR:HA	1:11:A:TRP:HD1	6	0.11	0.0	0.11
(2,336)	1:8:A:TYR:HA	1:11:A:TRP:HD1	6	0.11	0.0	0.11
(1,275)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.8	0.01	0.8
(2,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.8	0.01	0.8
(1,316)	1:1:A:GLU:HA	1:1:A:GLU:HG2	5	0.23	0.02	0.22
(2,287)	1:1:A:GLU:HA	1:1:A:GLU:HG2	5	0.23	0.02	0.22
(1,578)	1:24:A:PRO:HG2	1:25:A:SER:H	5	0.14	0.02	0.15
(2,508)	1:24:A:PRO:HG2	1:25:A:SER:H	5	0.14	0.02	0.15
(1,602)	1:2:A:GLU:HB2	1:5:A:VAL:H	5	0.13	0.02	0.13
(2,530)	1:2:A:GLU:HB2	1:5:A:VAL:H	5	0.13	0.02	0.13
(1,637)	1:2:A:GLU:HA	1:3:A:GLU:HB2	5	0.12	0.03	0.12
(2,565)	1:2:A:GLU:HA	1:3:A:GLU:HB2	5	0.12	0.03	0.12
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB2	5	0.11	0.01	0.11
(2,179)	1:17:A:PRO:HA	1:17:A:PRO:HB2	5	0.11	0.01	0.11
(1,516)	1:9:A:ILE:HG21	1:13:A:LYS:H	5	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,516)	1:9:A:ILE:HG22	1:13:A:LYS:H	5	0.11	0.0	0.11
(1,516)	1:9:A:ILE:HG23	1:13:A:LYS:H	5	0.11	0.0	0.11
(2,455)	1:9:A:ILE:HG21	1:13:A:LYS:H	5	0.11	0.0	0.11
(2,455)	1:9:A:ILE:HG22	1:13:A:LYS:H	5	0.11	0.0	0.11
(2,455)	1:9:A:ILE:HG23	1:13:A:LYS:H	5	0.11	0.0	0.11
(1,674)	1:14:A:ASP:HB2	1:19:A:SER:HB3	4	0.13	0.01	0.14
(2,600)	1:14:A:ASP:HB2	1:19:A:SER:HB3	4	0.13	0.01	0.14
(1,693)	1:2:A:GLU:HB3	1:6:A:ARG:HG3	4	0.11	0.01	0.11
(2,619)	1:2:A:GLU:HB3	1:6:A:ARG:HG3	4	0.11	0.01	0.11
(1,233)	1:21:A:ARG:H	1:21:A:ARG:HD2	3	0.2	0.13	0.11
(2,208)	1:21:A:ARG:H	1:21:A:ARG:HD2	3	0.2	0.13	0.11
(1,585)	1:24:A:PRO:HD3	1:25:A:SER:H	3	0.19	0.03	0.2
(2,514)	1:24:A:PRO:HD3	1:25:A:SER:H	3	0.19	0.03	0.2
(1,391)	1:11:A:TRP:HH2	1:22:A:PRO:HA	3	0.12	0.01	0.12
(2,349)	1:11:A:TRP:HH2	1:22:A:PRO:HA	3	0.12	0.01	0.12
(1,580)	1:24:A:PRO:HB2	1:25:A:SER:H	3	0.12	0.01	0.11
(2,509)	1:24:A:PRO:HB2	1:25:A:SER:H	3	0.12	0.01	0.11
(1,362)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	3	0.11	0.0	0.11
(2,322)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	3	0.11	0.0	0.11
(1,347)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	3	0.11	0.01	0.11
(1,347)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	3	0.11	0.01	0.11
(1,347)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	3	0.11	0.01	0.11
(1,347)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	3	0.11	0.01	0.11
(1,347)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	3	0.11	0.01	0.11
(1,347)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	3	0.11	0.01	0.11
(2,312)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	3	0.11	0.01	0.11
(2,312)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	3	0.11	0.01	0.11
(2,312)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	3	0.11	0.01	0.11
(2,312)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	3	0.11	0.01	0.11
(2,312)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	3	0.11	0.01	0.11
(2,312)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	3	0.11	0.01	0.11
(1,403)	1:14:A:ASP:HB2	1:21:A:ARG:HH11	2	0.14	0.01	0.14
(1,403)	1:14:A:ASP:HB2	1:21:A:ARG:HH12	2	0.14	0.01	0.14
(2,360)	1:14:A:ASP:HB2	1:21:A:ARG:HH11	2	0.14	0.01	0.14
(2,360)	1:14:A:ASP:HB2	1:21:A:ARG:HH12	2	0.14	0.01	0.14
(1,734)	1:6:A:ARG:HG3	1:7:A:LEU:HD11	2	0.13	0.03	0.13
(1,734)	1:6:A:ARG:HG3	1:7:A:LEU:HD12	2	0.13	0.03	0.13
(1,734)	1:6:A:ARG:HG3	1:7:A:LEU:HD13	2	0.13	0.03	0.13
(2,656)	1:6:A:ARG:HG3	1:7:A:LEU:HD11	2	0.13	0.03	0.13
(2,656)	1:6:A:ARG:HG3	1:7:A:LEU:HD12	2	0.13	0.03	0.13
(2,656)	1:6:A:ARG:HG3	1:7:A:LEU:HD13	2	0.13	0.03	0.13
(1,660)	1:1:A:GLU:HA	1:2:A:GLU:HB3	2	0.12	0.0	0.12

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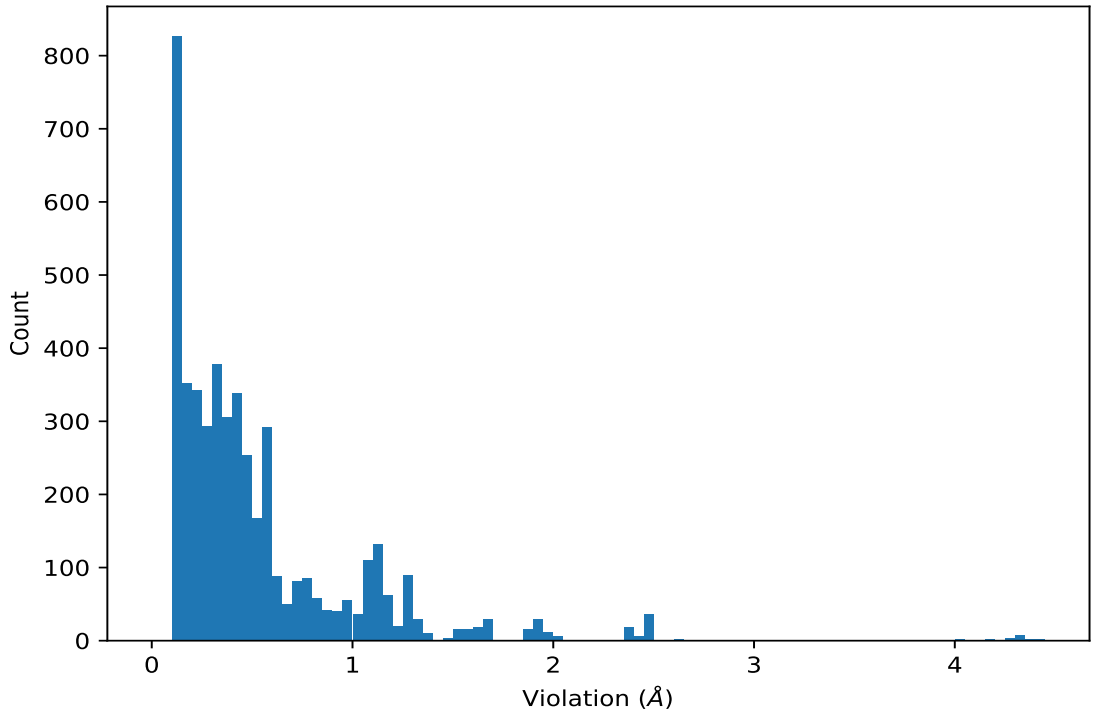
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,587)	1:1:A:GLU:HA	1:2:A:GLU:HB3	2	0.12	0.0	0.12
(1,392)	1:11:A:TRP:HH2	1:17:A:PRO:HA	2	0.11	0.0	0.11
(2,350)	1:11:A:TRP:HH2	1:17:A:PRO:HA	2	0.11	0.0	0.11
(1,575)	1:9:A:ILE:HG21	1:10:A:GLN:H	2	0.1	0.0	0.1
(1,575)	1:9:A:ILE:HG22	1:10:A:GLN:H	2	0.1	0.0	0.1
(1,575)	1:9:A:ILE:HG23	1:10:A:GLN:H	2	0.1	0.0	0.1
(1,724)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	2	0.1	0.0	0.1
(1,724)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	2	0.1	0.0	0.1
(1,724)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	2	0.1	0.0	0.1
(2,506)	1:9:A:ILE:HG21	1:10:A:GLN:H	2	0.1	0.0	0.1
(2,506)	1:9:A:ILE:HG22	1:10:A:GLN:H	2	0.1	0.0	0.1
(2,506)	1:9:A:ILE:HG23	1:10:A:GLN:H	2	0.1	0.0	0.1
(2,648)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	2	0.1	0.0	0.1
(2,648)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	2	0.1	0.0	0.1
(2,648)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	2	0.1	0.0	0.1

[1]Number of violated models, [2]Standard 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)
(3,29)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	10	4.42
(1,311)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	10	4.42
(3,29)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	7	4.37
(1,311)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	7	4.37
(3,29)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	4	4.34
(3,29)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	6	4.34
(1,311)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	4	4.34
(1,311)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	6	4.34
(3,29)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	3	4.32
(3,29)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	8	4.32
(1,311)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	3	4.32
(1,311)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	8	4.32
(3,29)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	2	4.28
(1,311)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	2	4.28
(3,29)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	9	4.25
(1,311)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	9	4.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,29)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	1	4.18
(1,311)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	1	4.18
(3,29)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	5	4.03
(1,311)	1:21:A:ARG:HG2	1:24:A:PRO:HG2	5	4.03
(2,697)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	4	2.62
(1,778)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	4	2.62
(3,84)	1:5:A:VAL:HG11	1:9:A:ILE:HB	5	2.48
(3,84)	1:5:A:VAL:HG12	1:9:A:ILE:HB	5	2.48
(3,84)	1:5:A:VAL:HG13	1:9:A:ILE:HB	5	2.48
(1,787)	1:5:A:VAL:HG11	1:9:A:ILE:HB	5	2.48
(1,787)	1:5:A:VAL:HG12	1:9:A:ILE:HB	5	2.48
(1,787)	1:5:A:VAL:HG13	1:9:A:ILE:HB	5	2.48
(3,84)	1:5:A:VAL:HG11	1:9:A:ILE:HB	10	2.47
(3,84)	1:5:A:VAL:HG12	1:9:A:ILE:HB	10	2.47
(3,84)	1:5:A:VAL:HG13	1:9:A:ILE:HB	10	2.47
(1,787)	1:5:A:VAL:HG11	1:9:A:ILE:HB	10	2.47
(1,787)	1:5:A:VAL:HG12	1:9:A:ILE:HB	10	2.47
(1,787)	1:5:A:VAL:HG13	1:9:A:ILE:HB	10	2.47
(3,84)	1:5:A:VAL:HG11	1:9:A:ILE:HB	1	2.46
(3,84)	1:5:A:VAL:HG12	1:9:A:ILE:HB	1	2.46
(3,84)	1:5:A:VAL:HG13	1:9:A:ILE:HB	1	2.46
(3,84)	1:5:A:VAL:HG11	1:9:A:ILE:HB	8	2.46
(3,84)	1:5:A:VAL:HG12	1:9:A:ILE:HB	8	2.46
(3,84)	1:5:A:VAL:HG13	1:9:A:ILE:HB	8	2.46
(1,787)	1:5:A:VAL:HG11	1:9:A:ILE:HB	1	2.46
(1,787)	1:5:A:VAL:HG12	1:9:A:ILE:HB	1	2.46
(1,787)	1:5:A:VAL:HG13	1:9:A:ILE:HB	1	2.46
(1,787)	1:5:A:VAL:HG11	1:9:A:ILE:HB	8	2.46
(1,787)	1:5:A:VAL:HG12	1:9:A:ILE:HB	8	2.46
(1,787)	1:5:A:VAL:HG13	1:9:A:ILE:HB	8	2.46
(3,84)	1:5:A:VAL:HG11	1:9:A:ILE:HB	3	2.45
(3,84)	1:5:A:VAL:HG12	1:9:A:ILE:HB	3	2.45
(3,84)	1:5:A:VAL:HG13	1:9:A:ILE:HB	3	2.45
(3,84)	1:5:A:VAL:HG11	1:9:A:ILE:HB	7	2.45
(3,84)	1:5:A:VAL:HG12	1:9:A:ILE:HB	7	2.45
(3,84)	1:5:A:VAL:HG13	1:9:A:ILE:HB	7	2.45
(1,787)	1:5:A:VAL:HG11	1:9:A:ILE:HB	3	2.45
(1,787)	1:5:A:VAL:HG12	1:9:A:ILE:HB	3	2.45
(1,787)	1:5:A:VAL:HG13	1:9:A:ILE:HB	3	2.45
(1,787)	1:5:A:VAL:HG11	1:9:A:ILE:HB	7	2.45
(1,787)	1:5:A:VAL:HG12	1:9:A:ILE:HB	7	2.45
(1,787)	1:5:A:VAL:HG13	1:9:A:ILE:HB	7	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,84)	1:5:A:VAL:HG11	1:9:A:ILE:HB	2	2.42
(3,84)	1:5:A:VAL:HG12	1:9:A:ILE:HB	2	2.42
(3,84)	1:5:A:VAL:HG13	1:9:A:ILE:HB	2	2.42
(1,787)	1:5:A:VAL:HG11	1:9:A:ILE:HB	2	2.42
(1,787)	1:5:A:VAL:HG12	1:9:A:ILE:HB	2	2.42
(1,787)	1:5:A:VAL:HG13	1:9:A:ILE:HB	2	2.42
(3,84)	1:5:A:VAL:HG11	1:9:A:ILE:HB	9	2.4
(3,84)	1:5:A:VAL:HG12	1:9:A:ILE:HB	9	2.4
(3,84)	1:5:A:VAL:HG13	1:9:A:ILE:HB	9	2.4
(1,787)	1:5:A:VAL:HG11	1:9:A:ILE:HB	9	2.4
(1,787)	1:5:A:VAL:HG12	1:9:A:ILE:HB	9	2.4
(1,787)	1:5:A:VAL:HG13	1:9:A:ILE:HB	9	2.4
(3,84)	1:5:A:VAL:HG11	1:9:A:ILE:HB	4	2.39
(3,84)	1:5:A:VAL:HG12	1:9:A:ILE:HB	4	2.39
(3,84)	1:5:A:VAL:HG13	1:9:A:ILE:HB	4	2.39
(1,787)	1:5:A:VAL:HG11	1:9:A:ILE:HB	4	2.39
(1,787)	1:5:A:VAL:HG12	1:9:A:ILE:HB	4	2.39
(1,787)	1:5:A:VAL:HG13	1:9:A:ILE:HB	4	2.39
(3,84)	1:5:A:VAL:HG11	1:9:A:ILE:HB	6	2.36
(3,84)	1:5:A:VAL:HG12	1:9:A:ILE:HB	6	2.36
(3,84)	1:5:A:VAL:HG13	1:9:A:ILE:HB	6	2.36
(1,787)	1:5:A:VAL:HG11	1:9:A:ILE:HB	6	2.36
(1,787)	1:5:A:VAL:HG12	1:9:A:ILE:HB	6	2.36
(1,787)	1:5:A:VAL:HG13	1:9:A:ILE:HB	6	2.36
(3,77)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	10	2.0
(3,77)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	10	2.0
(3,77)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	10	2.0
(1,725)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	10	2.0
(1,725)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	10	2.0
(1,725)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	10	2.0
(3,77)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	4	1.99
(3,77)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	4	1.99
(3,77)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	4	1.99
(1,725)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	4	1.99
(1,725)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	4	1.99
(1,725)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	4	1.99
(3,77)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	2	1.96
(3,77)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	2	1.96
(3,77)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	2	1.96
(1,725)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	2	1.96
(1,725)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	2	1.96
(1,725)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	2	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,77)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	8	1.94
(3,77)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	8	1.94
(3,77)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	8	1.94
(1,725)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	8	1.94
(1,725)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	8	1.94
(1,725)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	8	1.94
(3,77)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	1	1.93
(3,77)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	1	1.93
(3,77)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	1	1.93
(3,77)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	5	1.93
(3,77)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	5	1.93
(3,77)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	5	1.93
(1,725)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	1	1.93
(1,725)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	1	1.93
(1,725)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	1	1.93
(1,725)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	5	1.93
(1,725)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	5	1.93
(1,725)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	5	1.93
(3,77)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	3	1.92
(3,77)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	3	1.92
(3,77)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	3	1.92
(3,77)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	9	1.92
(3,77)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	9	1.92
(3,77)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	9	1.92
(1,725)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	3	1.92
(1,725)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	3	1.92
(1,725)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	3	1.92
(1,725)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	9	1.92
(1,725)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	9	1.92
(1,725)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	9	1.92
(3,77)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	7	1.9
(3,77)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	7	1.9
(3,77)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	7	1.9
(3,58)	1:3:A:GLU:HB3	1:7:A:LEU:H	6	1.9
(3,58)	1:3:A:GLU:HB3	1:7:A:LEU:H	9	1.9
(1,725)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	7	1.9
(1,725)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	7	1.9
(1,725)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	7	1.9
(1,495)	1:3:A:GLU:HB3	1:7:A:LEU:H	6	1.9
(1,495)	1:3:A:GLU:HB3	1:7:A:LEU:H	9	1.9
(3,77)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	6	1.86
(3,77)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	6	1.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,77)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	6	1.86
(1,725)	1:7:A:LEU:HD11	1:24:A:PRO:HB2	6	1.86
(1,725)	1:7:A:LEU:HD12	1:24:A:PRO:HB2	6	1.86
(1,725)	1:7:A:LEU:HD13	1:24:A:PRO:HB2	6	1.86
(3,58)	1:3:A:GLU:HB3	1:7:A:LEU:H	5	1.7
(3,49)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	2	1.7
(3,49)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	2	1.7
(3,49)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	10	1.7
(3,49)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	10	1.7
(1,495)	1:3:A:GLU:HB3	1:7:A:LEU:H	5	1.7
(1,459)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	2	1.7
(1,459)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	2	1.7
(1,459)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	10	1.7
(1,459)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	10	1.7
(3,49)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	8	1.69
(3,49)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	8	1.69
(1,459)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	8	1.69
(1,459)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	8	1.69
(3,49)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	4	1.68
(3,49)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	4	1.68
(1,459)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	4	1.68
(1,459)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	4	1.68
(3,58)	1:3:A:GLU:HB3	1:7:A:LEU:H	2	1.67
(3,49)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	9	1.67
(3,49)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	9	1.67
(1,495)	1:3:A:GLU:HB3	1:7:A:LEU:H	2	1.67
(1,459)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	9	1.67
(1,459)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	9	1.67
(3,58)	1:3:A:GLU:HB3	1:7:A:LEU:H	1	1.66
(3,49)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	1	1.66
(3,49)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	1	1.66
(1,495)	1:3:A:GLU:HB3	1:7:A:LEU:H	1	1.66
(1,459)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	1	1.66
(1,459)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	1	1.66
(3,49)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	3	1.65
(3,49)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	3	1.65
(3,49)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	7	1.65
(3,49)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	7	1.65
(1,459)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	3	1.65
(1,459)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	3	1.65
(1,459)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	7	1.65
(1,459)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	7	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,58)	1:3:A:GLU:HB3	1:7:A:LEU:H	10	1.64
(3,49)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	6	1.64
(3,49)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	6	1.64
(1,495)	1:3:A:GLU:HB3	1:7:A:LEU:H	10	1.64
(1,459)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	6	1.64
(1,459)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	6	1.64
(3,58)	1:3:A:GLU:HB3	1:7:A:LEU:H	3	1.61
(1,495)	1:3:A:GLU:HB3	1:7:A:LEU:H	3	1.61
(3,58)	1:3:A:GLU:HB3	1:7:A:LEU:H	8	1.6
(1,495)	1:3:A:GLU:HB3	1:7:A:LEU:H	8	1.6
(2,683)	1:14:A:ASP:HB2	1:19:A:SER:HA	5	1.58
(1,763)	1:14:A:ASP:HB2	1:19:A:SER:HA	5	1.58
(3,58)	1:3:A:GLU:HB3	1:7:A:LEU:H	7	1.57
(3,49)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	5	1.57
(3,49)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	5	1.57
(2,683)	1:14:A:ASP:HB2	1:19:A:SER:HA	7	1.57
(1,763)	1:14:A:ASP:HB2	1:19:A:SER:HA	7	1.57
(1,495)	1:3:A:GLU:HB3	1:7:A:LEU:H	7	1.57
(1,459)	1:8:A:TYR:HD1	1:11:A:TRP:HH2	5	1.57
(1,459)	1:8:A:TYR:HD2	1:11:A:TRP:HH2	5	1.57
(3,72)	1:3:A:GLU:HG2	1:5:A:VAL:H	4	1.56
(2,683)	1:14:A:ASP:HB2	1:19:A:SER:HA	9	1.56
(2,683)	1:14:A:ASP:HB2	1:19:A:SER:HA	10	1.56
(1,763)	1:14:A:ASP:HB2	1:19:A:SER:HA	9	1.56
(1,763)	1:14:A:ASP:HB2	1:19:A:SER:HA	10	1.56
(1,599)	1:3:A:GLU:HG2	1:5:A:VAL:H	4	1.56
(3,58)	1:3:A:GLU:HB3	1:7:A:LEU:H	4	1.54
(2,507)	1:23:A:PRO:HB3	1:25:A:SER:H	7	1.54
(1,577)	1:23:A:PRO:HB3	1:25:A:SER:H	7	1.54
(1,495)	1:3:A:GLU:HB3	1:7:A:LEU:H	4	1.54
(2,683)	1:14:A:ASP:HB2	1:19:A:SER:HA	3	1.53
(1,763)	1:14:A:ASP:HB2	1:19:A:SER:HA	3	1.53
(2,683)	1:14:A:ASP:HB2	1:19:A:SER:HA	1	1.52
(2,683)	1:14:A:ASP:HB2	1:19:A:SER:HA	2	1.52
(2,507)	1:23:A:PRO:HB3	1:25:A:SER:H	6	1.52
(1,763)	1:14:A:ASP:HB2	1:19:A:SER:HA	1	1.52
(1,763)	1:14:A:ASP:HB2	1:19:A:SER:HA	2	1.52
(1,577)	1:23:A:PRO:HB3	1:25:A:SER:H	6	1.52
(2,683)	1:14:A:ASP:HB2	1:19:A:SER:HA	4	1.51
(1,763)	1:14:A:ASP:HB2	1:19:A:SER:HA	4	1.51
(2,507)	1:23:A:PRO:HB3	1:25:A:SER:H	10	1.5
(1,577)	1:23:A:PRO:HB3	1:25:A:SER:H	10	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,683)	1:14:A:ASP:HB2	1:19:A:SER:HA	8	1.49
(1,763)	1:14:A:ASP:HB2	1:19:A:SER:HA	8	1.49
(2,683)	1:14:A:ASP:HB2	1:19:A:SER:HA	6	1.48
(1,763)	1:14:A:ASP:HB2	1:19:A:SER:HA	6	1.48
(2,368)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	7	1.38
(2,368)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	10	1.38
(1,411)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	7	1.38
(1,411)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	10	1.38
(3,73)	1:3:A:GLU:HA	1:7:A:LEU:HG	9	1.37
(2,697)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	8	1.37
(2,368)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	6	1.37
(1,778)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	8	1.37
(1,640)	1:3:A:GLU:HA	1:7:A:LEU:HG	9	1.37
(1,411)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	6	1.37
(3,68)	1:5:A:VAL:HB	1:6:A:ARG:H	8	1.34
(2,368)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	3	1.34
(2,368)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	9	1.34
(1,560)	1:5:A:VAL:HB	1:6:A:ARG:H	8	1.34
(1,411)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	3	1.34
(1,411)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	9	1.34
(3,73)	1:3:A:GLU:HA	1:7:A:LEU:HG	4	1.33
(3,68)	1:5:A:VAL:HB	1:6:A:ARG:H	5	1.33
(2,697)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	1	1.33
(2,697)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	5	1.33
(1,778)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	1	1.33
(1,778)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	5	1.33
(1,640)	1:3:A:GLU:HA	1:7:A:LEU:HG	4	1.33
(1,560)	1:5:A:VAL:HB	1:6:A:ARG:H	5	1.33
(3,68)	1:5:A:VAL:HB	1:6:A:ARG:H	10	1.32
(1,560)	1:5:A:VAL:HB	1:6:A:ARG:H	10	1.32
(3,68)	1:5:A:VAL:HB	1:6:A:ARG:H	1	1.31
(3,68)	1:5:A:VAL:HB	1:6:A:ARG:H	2	1.31
(3,68)	1:5:A:VAL:HB	1:6:A:ARG:H	3	1.31
(3,68)	1:5:A:VAL:HB	1:6:A:ARG:H	7	1.31
(1,560)	1:5:A:VAL:HB	1:6:A:ARG:H	1	1.31
(1,560)	1:5:A:VAL:HB	1:6:A:ARG:H	2	1.31
(1,560)	1:5:A:VAL:HB	1:6:A:ARG:H	3	1.31
(1,560)	1:5:A:VAL:HB	1:6:A:ARG:H	7	1.31
(2,697)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	2	1.3
(2,697)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	10	1.3
(2,368)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	4	1.3
(1,778)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	2	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	10	1.3
(1,411)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	4	1.3
(3,73)	1:3:A:GLU:HA	1:7:A:LEU:HG	6	1.29
(3,68)	1:5:A:VAL:HB	1:6:A:ARG:H	9	1.29
(2,697)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	3	1.29
(2,697)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	6	1.29
(2,368)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	1	1.29
(1,778)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	3	1.29
(1,778)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	6	1.29
(1,640)	1:3:A:GLU:HA	1:7:A:LEU:HG	6	1.29
(1,560)	1:5:A:VAL:HB	1:6:A:ARG:H	9	1.29
(1,411)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	1	1.29
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	6	1.28
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	6	1.28
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	6	1.28
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	6	1.28
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	6	1.28
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	6	1.28
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	6	1.28
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	6	1.28
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	6	1.28
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	6	1.28
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	6	1.28
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	6	1.28
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	8	1.27
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	8	1.27
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	8	1.27
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	8	1.27
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	8	1.27
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	8	1.27
(2,697)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	7	1.27
(2,368)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	5	1.27
(1,778)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	7	1.27
(1,411)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	5	1.27
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	8	1.27
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	8	1.27
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	8	1.27
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	8	1.27
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	8	1.27
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	8	1.27
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	2	1.26
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	2	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	2	1.26
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	2	1.26
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	2	1.26
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	2	1.26
(2,368)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	2	1.26
(1,411)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	2	1.26
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	2	1.26
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	2	1.26
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	2	1.26
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	2	1.26
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	2	1.26
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	2	1.26
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	5	1.25
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	5	1.25
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	5	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	5	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	5	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	5	1.25
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	9	1.25
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	9	1.25
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	9	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	9	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	9	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	9	1.25
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	10	1.25
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	10	1.25
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	10	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	10	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	10	1.25
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	10	1.25
(2,368)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	8	1.25
(1,411)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	8	1.25
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	5	1.25
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	5	1.25
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	5	1.25
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	5	1.25
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	5	1.25
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	5	1.25
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	9	1.25
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	9	1.25
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	9	1.25
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	9	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	9	1.25
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	9	1.25
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	10	1.25
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	10	1.25
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	10	1.25
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	10	1.25
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	10	1.25
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	10	1.25
(3,68)	1:5:A:VAL:HB	1:6:A:ARG:H	4	1.24
(3,68)	1:5:A:VAL:HB	1:6:A:ARG:H	6	1.24
(1,560)	1:5:A:VAL:HB	1:6:A:ARG:H	4	1.24
(1,560)	1:5:A:VAL:HB	1:6:A:ARG:H	6	1.24
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	7	1.23
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	7	1.23
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	7	1.23
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	7	1.23
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	7	1.23
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	7	1.23
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	7	1.23
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	7	1.23
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	7	1.23
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	7	1.23
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	7	1.23
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	7	1.23
(3,73)	1:3:A:GLU:HA	1:7:A:LEU:HG	7	1.22
(3,73)	1:3:A:GLU:HA	1:7:A:LEU:HG	10	1.22
(1,640)	1:3:A:GLU:HA	1:7:A:LEU:HG	7	1.22
(1,640)	1:3:A:GLU:HA	1:7:A:LEU:HG	10	1.22
(3,73)	1:3:A:GLU:HA	1:7:A:LEU:HG	5	1.2
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	4	1.2
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	4	1.2
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	4	1.2
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	4	1.2
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	4	1.2
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	4	1.2
(1,640)	1:3:A:GLU:HA	1:7:A:LEU:HG	5	1.2
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	4	1.2
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	4	1.2
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	4	1.2
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	4	1.2
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	4	1.2
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	4	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,507)	1:23:A:PRO:HB3	1:25:A:SER:H	3	1.19
(2,507)	1:23:A:PRO:HB3	1:25:A:SER:H	4	1.19
(2,338)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	6	1.19
(1,577)	1:23:A:PRO:HB3	1:25:A:SER:H	3	1.19
(1,577)	1:23:A:PRO:HB3	1:25:A:SER:H	4	1.19
(1,378)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	6	1.19
(2,338)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	3	1.18
(2,338)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	4	1.18
(2,338)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	8	1.18
(1,378)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	3	1.18
(1,378)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	4	1.18
(1,378)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	8	1.18
(3,73)	1:3:A:GLU:HA	1:7:A:LEU:HG	3	1.17
(3,60)	1:4:A:ALA:H	1:7:A:LEU:HB3	7	1.17
(3,60)	1:4:A:ALA:H	1:7:A:LEU:HB3	10	1.17
(3,44)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	1.17
(2,697)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	9	1.17
(2,374)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	6	1.17
(2,374)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	7	1.17
(1,778)	1:3:A:GLU:HG2	1:6:A:ARG:HB3	9	1.17
(1,640)	1:3:A:GLU:HA	1:7:A:LEU:HG	3	1.17
(1,499)	1:4:A:ALA:H	1:7:A:LEU:HB3	7	1.17
(1,499)	1:4:A:ALA:H	1:7:A:LEU:HB3	10	1.17
(1,423)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	1.17
(1,417)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	6	1.17
(1,417)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	7	1.17
(3,44)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	1.16
(3,44)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	1.16
(3,44)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	1.16
(3,44)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	1.16
(3,44)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	1.16
(3,44)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	1.16
(3,44)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.16
(2,374)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	2	1.16
(2,374)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	3	1.16
(2,374)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	1.16
(2,338)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	9	1.16
(1,423)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	1.16
(1,423)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	1.16
(1,423)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	1.16
(1,423)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	1.16
(1,423)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	1.16
(1,423)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.16
(1,417)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	2	1.16
(1,417)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	3	1.16
(1,417)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	1.16
(1,378)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	9	1.16
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	5	1.15
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	5	1.15
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	5	1.15
(3,60)	1:4:A:ALA:H	1:7:A:LEU:HB3	2	1.15
(3,60)	1:4:A:ALA:H	1:7:A:LEU:HB3	3	1.15
(3,60)	1:4:A:ALA:H	1:7:A:LEU:HB3	4	1.15
(3,60)	1:4:A:ALA:H	1:7:A:LEU:HB3	9	1.15
(3,44)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	1.15
(3,44)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	1.15
(2,374)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	1	1.15
(2,374)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	9	1.15
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	5	1.15
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	5	1.15
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	5	1.15
(1,499)	1:4:A:ALA:H	1:7:A:LEU:HB3	2	1.15
(1,499)	1:4:A:ALA:H	1:7:A:LEU:HB3	3	1.15
(1,499)	1:4:A:ALA:H	1:7:A:LEU:HB3	4	1.15
(1,499)	1:4:A:ALA:H	1:7:A:LEU:HB3	9	1.15
(1,423)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	1.15
(1,423)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	1.15
(1,417)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	1	1.15
(1,417)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	9	1.15
(3,73)	1:3:A:GLU:HA	1:7:A:LEU:HG	2	1.14
(3,60)	1:4:A:ALA:H	1:7:A:LEU:HB3	1	1.14
(3,60)	1:4:A:ALA:H	1:7:A:LEU:HB3	5	1.14
(2,374)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	8	1.14
(1,640)	1:3:A:GLU:HA	1:7:A:LEU:HG	2	1.14
(1,499)	1:4:A:ALA:H	1:7:A:LEU:HB3	1	1.14
(1,499)	1:4:A:ALA:H	1:7:A:LEU:HB3	5	1.14
(1,417)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	8	1.14
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	7	1.13
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	7	1.13
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	7	1.13
(3,61)	1:5:A:VAL:HG11	1:9:A:ILE:H	1	1.13
(3,61)	1:5:A:VAL:HG12	1:9:A:ILE:H	1	1.13
(3,61)	1:5:A:VAL:HG13	1:9:A:ILE:H	1	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,60)	1:4:A:ALA:H	1:7:A:LEU:HB3	8	1.13
(3,51)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	2	1.13
(3,51)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	2	1.13
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	3	1.13
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	3	1.13
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	3	1.13
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	3	1.13
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	3	1.13
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	3	1.13
(2,374)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	4	1.13
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	7	1.13
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	7	1.13
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	7	1.13
(1,504)	1:5:A:VAL:HG11	1:9:A:ILE:H	1	1.13
(1,504)	1:5:A:VAL:HG12	1:9:A:ILE:H	1	1.13
(1,504)	1:5:A:VAL:HG13	1:9:A:ILE:H	1	1.13
(1,499)	1:4:A:ALA:H	1:7:A:LEU:HB3	8	1.13
(1,461)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	2	1.13
(1,461)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	2	1.13
(1,417)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	4	1.13
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	3	1.13
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	3	1.13
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	3	1.13
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	3	1.13
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	3	1.13
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	3	1.13
(3,61)	1:5:A:VAL:HG11	1:9:A:ILE:H	3	1.12
(3,61)	1:5:A:VAL:HG12	1:9:A:ILE:H	3	1.12
(3,61)	1:5:A:VAL:HG13	1:9:A:ILE:H	3	1.12
(3,61)	1:5:A:VAL:HG11	1:9:A:ILE:H	5	1.12
(3,61)	1:5:A:VAL:HG12	1:9:A:ILE:H	5	1.12
(3,61)	1:5:A:VAL:HG13	1:9:A:ILE:H	5	1.12
(3,61)	1:5:A:VAL:HG11	1:9:A:ILE:H	8	1.12
(3,61)	1:5:A:VAL:HG12	1:9:A:ILE:H	8	1.12
(3,61)	1:5:A:VAL:HG13	1:9:A:ILE:H	8	1.12
(3,61)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	1.12
(3,61)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	1.12
(3,61)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	1.12
(3,51)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	8	1.12
(3,51)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	8	1.12
(3,51)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	9	1.12
(3,51)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	9	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,374)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	5	1.12
(1,504)	1:5:A:VAL:HG11	1:9:A:ILE:H	3	1.12
(1,504)	1:5:A:VAL:HG12	1:9:A:ILE:H	3	1.12
(1,504)	1:5:A:VAL:HG13	1:9:A:ILE:H	3	1.12
(1,504)	1:5:A:VAL:HG11	1:9:A:ILE:H	5	1.12
(1,504)	1:5:A:VAL:HG12	1:9:A:ILE:H	5	1.12
(1,504)	1:5:A:VAL:HG13	1:9:A:ILE:H	5	1.12
(1,504)	1:5:A:VAL:HG11	1:9:A:ILE:H	8	1.12
(1,504)	1:5:A:VAL:HG12	1:9:A:ILE:H	8	1.12
(1,504)	1:5:A:VAL:HG13	1:9:A:ILE:H	8	1.12
(1,504)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	1.12
(1,504)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	1.12
(1,504)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	1.12
(1,461)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	8	1.12
(1,461)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	8	1.12
(1,461)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	9	1.12
(1,461)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	9	1.12
(1,417)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	5	1.12
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	10	1.11
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	10	1.11
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	10	1.11
(3,61)	1:5:A:VAL:HG11	1:9:A:ILE:H	2	1.11
(3,61)	1:5:A:VAL:HG12	1:9:A:ILE:H	2	1.11
(3,61)	1:5:A:VAL:HG13	1:9:A:ILE:H	2	1.11
(3,61)	1:5:A:VAL:HG11	1:9:A:ILE:H	7	1.11
(3,61)	1:5:A:VAL:HG12	1:9:A:ILE:H	7	1.11
(3,61)	1:5:A:VAL:HG13	1:9:A:ILE:H	7	1.11
(3,60)	1:4:A:ALA:H	1:7:A:LEU:HB3	6	1.11
(3,51)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	10	1.11
(3,51)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	10	1.11
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	10	1.11
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	10	1.11
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	10	1.11
(1,504)	1:5:A:VAL:HG11	1:9:A:ILE:H	2	1.11
(1,504)	1:5:A:VAL:HG12	1:9:A:ILE:H	2	1.11
(1,504)	1:5:A:VAL:HG13	1:9:A:ILE:H	2	1.11
(1,504)	1:5:A:VAL:HG11	1:9:A:ILE:H	7	1.11
(1,504)	1:5:A:VAL:HG12	1:9:A:ILE:H	7	1.11
(1,504)	1:5:A:VAL:HG13	1:9:A:ILE:H	7	1.11
(1,499)	1:4:A:ALA:H	1:7:A:LEU:HB3	6	1.11
(1,461)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	10	1.11
(1,461)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	10	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	8	1.1
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	8	1.1
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	8	1.1
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	2	1.1
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	2	1.1
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	2	1.1
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	8	1.1
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	8	1.1
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	8	1.1
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	2	1.1
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	2	1.1
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	2	1.1
(3,61)	1:5:A:VAL:HG11	1:9:A:ILE:H	4	1.09
(3,61)	1:5:A:VAL:HG12	1:9:A:ILE:H	4	1.09
(3,61)	1:5:A:VAL:HG13	1:9:A:ILE:H	4	1.09
(3,51)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	4	1.09
(3,51)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	4	1.09
(2,342)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	2	1.09
(1,504)	1:5:A:VAL:HG11	1:9:A:ILE:H	4	1.09
(1,504)	1:5:A:VAL:HG12	1:9:A:ILE:H	4	1.09
(1,504)	1:5:A:VAL:HG13	1:9:A:ILE:H	4	1.09
(1,461)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	4	1.09
(1,461)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	4	1.09
(1,383)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	2	1.09
(3,61)	1:5:A:VAL:HG11	1:9:A:ILE:H	9	1.08
(3,61)	1:5:A:VAL:HG12	1:9:A:ILE:H	9	1.08
(3,61)	1:5:A:VAL:HG13	1:9:A:ILE:H	9	1.08
(3,51)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	1	1.08
(3,51)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	1	1.08
(3,51)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	7	1.08
(3,51)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	7	1.08
(3,3)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	1.08
(2,342)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	1	1.08
(2,342)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	4	1.08
(2,342)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	8	1.08
(1,504)	1:5:A:VAL:HG11	1:9:A:ILE:H	9	1.08
(1,504)	1:5:A:VAL:HG12	1:9:A:ILE:H	9	1.08
(1,504)	1:5:A:VAL:HG13	1:9:A:ILE:H	9	1.08
(1,461)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	1	1.08
(1,461)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	1	1.08
(1,461)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	7	1.08
(1,461)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	7	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	1	1.08
(1,383)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	4	1.08
(1,383)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	8	1.08
(1,15)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	1.08
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	2	1.07
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	2	1.07
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	2	1.07
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	6	1.07
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	6	1.07
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	6	1.07
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	9	1.07
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	9	1.07
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	9	1.07
(3,51)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	3	1.07
(3,51)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	3	1.07
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	1	1.07
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	1	1.07
(3,34)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	1	1.07
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	1	1.07
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	1	1.07
(3,34)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	1	1.07
(2,696)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	3	1.07
(2,696)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	6	1.07
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	1	1.07
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	1	1.07
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	1	1.07
(2,342)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	6	1.07
(1,777)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	3	1.07
(1,777)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	6	1.07
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	2	1.07
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	2	1.07
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	2	1.07
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	6	1.07
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	6	1.07
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	6	1.07
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	9	1.07
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	9	1.07
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	9	1.07
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	1	1.07
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	1	1.07
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	1	1.07
(1,461)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	3	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	3	1.07
(1,383)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	6	1.07
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	1	1.07
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	1	1.07
(1,341)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	1	1.07
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	1	1.07
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	1	1.07
(1,341)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	1	1.07
(3,61)	1:5:A:VAL:HG11	1:9:A:ILE:H	6	1.06
(3,61)	1:5:A:VAL:HG12	1:9:A:ILE:H	6	1.06
(3,61)	1:5:A:VAL:HG13	1:9:A:ILE:H	6	1.06
(3,51)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	6	1.06
(3,51)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	6	1.06
(3,4)	1:3:A:GLU:H	1:3:A:GLU:HG3	9	1.06
(2,696)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	2	1.06
(2,696)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	4	1.06
(2,338)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	7	1.06
(1,777)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	2	1.06
(1,777)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	4	1.06
(1,504)	1:5:A:VAL:HG11	1:9:A:ILE:H	6	1.06
(1,504)	1:5:A:VAL:HG12	1:9:A:ILE:H	6	1.06
(1,504)	1:5:A:VAL:HG13	1:9:A:ILE:H	6	1.06
(1,461)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	6	1.06
(1,461)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	6	1.06
(1,378)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	7	1.06
(1,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	9	1.06
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	4	1.05
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	4	1.05
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	4	1.05
(3,73)	1:3:A:GLU:HA	1:7:A:LEU:HG	1	1.05
(2,342)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	3	1.05
(2,338)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	10	1.05
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	4	1.05
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	4	1.05
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	4	1.05
(1,640)	1:3:A:GLU:HA	1:7:A:LEU:HG	1	1.05
(1,383)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	3	1.05
(1,378)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	10	1.05
(2,696)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	8	1.04
(2,338)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	2	1.04
(1,777)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	8	1.04
(1,378)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	2	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	3	1.03
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	3	1.03
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	3	1.03
(3,73)	1:3:A:GLU:HA	1:7:A:LEU:HG	8	1.03
(3,51)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	5	1.03
(3,51)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	5	1.03
(2,696)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	1	1.03
(2,615)	1:3:A:GLU:HG2	1:7:A:LEU:HG	4	1.03
(1,777)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	1	1.03
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	3	1.03
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	3	1.03
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	3	1.03
(1,689)	1:3:A:GLU:HG2	1:7:A:LEU:HG	4	1.03
(1,640)	1:3:A:GLU:HA	1:7:A:LEU:HG	8	1.03
(1,461)	1:8:A:TYR:HD1	1:11:A:TRP:HZ3	5	1.03
(1,461)	1:8:A:TYR:HD2	1:11:A:TRP:HZ3	5	1.03
(2,696)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	9	1.02
(2,696)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	10	1.02
(2,338)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	1	1.02
(1,777)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	9	1.02
(1,777)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	10	1.02
(1,378)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	1	1.02
(3,13)	1:7:A:LEU:H	1:7:A:LEU:HG	7	1.0
(2,696)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	7	1.0
(2,695)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	3	1.0
(2,584)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	1.0
(2,507)	1:23:A:PRO:HB3	1:25:A:SER:H	8	1.0
(1,777)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	7	1.0
(1,776)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	3	1.0
(1,657)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	1.0
(1,577)	1:23:A:PRO:HB3	1:25:A:SER:H	8	1.0
(1,81)	1:7:A:LEU:H	1:7:A:LEU:HG	7	1.0
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	1	0.99
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	1	0.99
(3,78)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	1	0.99
(2,695)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	4	0.99
(2,695)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	6	0.99
(2,617)	1:3:A:GLU:HG2	1:6:A:ARG:HG3	4	0.99
(1,776)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	4	0.99
(1,776)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	6	0.99
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	1	0.99
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	1	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,731)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	1	0.99
(1,691)	1:3:A:GLU:HG2	1:6:A:ARG:HG3	4	0.99
(3,3)	1:3:A:GLU:H	1:3:A:GLU:HG2	7	0.98
(3,3)	1:3:A:GLU:H	1:3:A:GLU:HG2	8	0.98
(2,695)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	2	0.98
(2,584)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	0.98
(2,584)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	0.98
(2,342)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	10	0.98
(1,776)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	2	0.98
(1,657)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	0.98
(1,657)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	0.98
(1,383)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	10	0.98
(1,15)	1:3:A:GLU:H	1:3:A:GLU:HG2	7	0.98
(1,15)	1:3:A:GLU:H	1:3:A:GLU:HG2	8	0.98
(3,13)	1:7:A:LEU:H	1:7:A:LEU:HG	9	0.97
(2,695)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	8	0.97
(2,584)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	1	0.97
(2,584)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	0.97
(2,342)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	5	0.97
(1,776)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	8	0.97
(1,657)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	1	0.97
(1,657)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	0.97
(1,383)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	5	0.97
(1,81)	1:7:A:LEU:H	1:7:A:LEU:HG	9	0.97
(3,13)	1:7:A:LEU:H	1:7:A:LEU:HG	3	0.96
(3,13)	1:7:A:LEU:H	1:7:A:LEU:HG	5	0.96
(3,13)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.96
(3,3)	1:3:A:GLU:H	1:3:A:GLU:HG2	3	0.96
(2,695)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	1	0.96
(2,695)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	9	0.96
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	6	0.96
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	6	0.96
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	6	0.96
(2,584)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	0.96
(2,584)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	0.96
(1,776)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	1	0.96
(1,776)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	9	0.96
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	6	0.96
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	6	0.96
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	6	0.96
(1,657)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	0.96
(1,657)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:7:A:LEU:H	1:7:A:LEU:HG	3	0.96
(1,81)	1:7:A:LEU:H	1:7:A:LEU:HG	5	0.96
(1,81)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.96
(1,15)	1:3:A:GLU:H	1:3:A:GLU:HG2	3	0.96
(3,13)	1:7:A:LEU:H	1:7:A:LEU:HG	4	0.95
(3,13)	1:7:A:LEU:H	1:7:A:LEU:HG	6	0.95
(3,3)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.95
(2,584)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	0.95
(2,584)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.95
(2,342)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	7	0.95
(1,657)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	0.95
(1,657)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.95
(1,383)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	7	0.95
(1,81)	1:7:A:LEU:H	1:7:A:LEU:HG	4	0.95
(1,81)	1:7:A:LEU:H	1:7:A:LEU:HG	6	0.95
(1,15)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.95
(3,13)	1:7:A:LEU:H	1:7:A:LEU:HG	1	0.94
(3,13)	1:7:A:LEU:H	1:7:A:LEU:HG	2	0.94
(3,3)	1:3:A:GLU:H	1:3:A:GLU:HG2	1	0.94
(3,3)	1:3:A:GLU:H	1:3:A:GLU:HG2	5	0.94
(2,695)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	10	0.94
(2,584)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	0.94
(1,776)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	10	0.94
(1,657)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	0.94
(1,81)	1:7:A:LEU:H	1:7:A:LEU:HG	1	0.94
(1,81)	1:7:A:LEU:H	1:7:A:LEU:HG	2	0.94
(1,15)	1:3:A:GLU:H	1:3:A:GLU:HG2	1	0.94
(1,15)	1:3:A:GLU:H	1:3:A:GLU:HG2	5	0.94
(3,13)	1:7:A:LEU:H	1:7:A:LEU:HG	8	0.93
(3,3)	1:3:A:GLU:H	1:3:A:GLU:HG2	2	0.93
(2,695)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	7	0.93
(2,338)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	5	0.93
(1,776)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	7	0.93
(1,378)	1:11:A:TRP:HD1	1:22:A:PRO:HD3	5	0.93
(1,81)	1:7:A:LEU:H	1:7:A:LEU:HG	8	0.93
(1,15)	1:3:A:GLU:H	1:3:A:GLU:HG2	2	0.93
(2,342)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	9	0.92
(1,383)	1:11:A:TRP:HD1	1:14:A:ASP:HB2	9	0.92
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	8	0.91
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	8	0.91
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	8	0.91
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	8	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	8	0.91
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	8	0.91
(3,41)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.89
(3,41)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.89
(1,382)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.89
(1,382)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.89
(3,41)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.88
(2,696)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	5	0.88
(2,507)	1:23:A:PRO:HB3	1:25:A:SER:H	2	0.88
(1,777)	1:8:A:TYR:HB2	1:24:A:PRO:HD3	5	0.88
(1,577)	1:23:A:PRO:HB3	1:25:A:SER:H	2	0.88
(1,382)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.88
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	6	0.87
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	6	0.87
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	6	0.87
(3,64)	1:21:A:ARG:H	1:22:A:PRO:HD2	5	0.87
(3,64)	1:21:A:ARG:H	1:22:A:PRO:HD2	10	0.87
(3,41)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.87
(3,41)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.87
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	6	0.87
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	6	0.87
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	6	0.87
(1,532)	1:21:A:ARG:H	1:22:A:PRO:HD2	5	0.87
(1,532)	1:21:A:ARG:H	1:22:A:PRO:HD2	10	0.87
(1,382)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.87
(1,382)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.87
(3,72)	1:3:A:GLU:HG2	1:5:A:VAL:H	7	0.86
(3,64)	1:21:A:ARG:H	1:22:A:PRO:HD2	1	0.86
(3,64)	1:21:A:ARG:H	1:22:A:PRO:HD2	7	0.86
(3,41)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	0.86
(3,41)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.86
(3,41)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.86
(3,41)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.86
(3,41)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	0.86
(3,3)	1:3:A:GLU:H	1:3:A:GLU:HG2	6	0.86
(1,599)	1:3:A:GLU:HG2	1:5:A:VAL:H	7	0.86
(1,532)	1:21:A:ARG:H	1:22:A:PRO:HD2	1	0.86
(1,532)	1:21:A:ARG:H	1:22:A:PRO:HD2	7	0.86
(1,382)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	0.86
(1,382)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.86
(1,382)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.86
(1,382)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	0.86
(1,15)	1:3:A:GLU:H	1:3:A:GLU:HG2	6	0.86
(3,64)	1:21:A:ARG:H	1:22:A:PRO:HD2	2	0.85
(1,532)	1:21:A:ARG:H	1:22:A:PRO:HD2	2	0.85
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	9	0.84
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	9	0.84
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	9	0.84
(2,695)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	5	0.84
(1,776)	1:8:A:TYR:HB3	1:24:A:PRO:HD3	5	0.84
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	9	0.84
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	9	0.84
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	9	0.84
(3,72)	1:3:A:GLU:HG2	1:5:A:VAL:H	8	0.83
(3,3)	1:3:A:GLU:H	1:3:A:GLU:HG2	9	0.83
(1,599)	1:3:A:GLU:HG2	1:5:A:VAL:H	8	0.83
(1,15)	1:3:A:GLU:H	1:3:A:GLU:HG2	9	0.83
(3,72)	1:3:A:GLU:HG2	1:5:A:VAL:H	3	0.82
(2,655)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	4	0.82
(2,655)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	4	0.82
(2,655)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	4	0.82
(2,214)	1:21:A:ARG:H	1:21:A:ARG:HG3	4	0.82
(2,214)	1:21:A:ARG:H	1:21:A:ARG:HG3	6	0.82
(1,733)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	4	0.82
(1,733)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	4	0.82
(1,733)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	4	0.82
(1,599)	1:3:A:GLU:HG2	1:5:A:VAL:H	3	0.82
(1,240)	1:21:A:ARG:H	1:21:A:ARG:HG3	4	0.82
(1,240)	1:21:A:ARG:H	1:21:A:ARG:HG3	6	0.82
(2,390)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	7	0.81
(2,390)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.81
(2,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.81
(2,214)	1:21:A:ARG:H	1:21:A:ARG:HG3	3	0.81
(2,214)	1:21:A:ARG:H	1:21:A:ARG:HG3	8	0.81
(2,214)	1:21:A:ARG:H	1:21:A:ARG:HG3	9	0.81
(1,434)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	7	0.81
(1,434)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.81
(1,275)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.81
(1,240)	1:21:A:ARG:H	1:21:A:ARG:HG3	3	0.81
(1,240)	1:21:A:ARG:H	1:21:A:ARG:HG3	8	0.81
(1,240)	1:21:A:ARG:H	1:21:A:ARG:HG3	9	0.81
(3,57)	1:3:A:GLU:HB2	1:7:A:LEU:H	3	0.8
(3,37)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	5	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,37)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	5	0.8
(2,390)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	6	0.8
(2,318)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	7	0.8
(2,318)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	7	0.8
(2,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	1	0.8
(2,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	7	0.8
(2,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	10	0.8
(2,214)	1:21:A:ARG:H	1:21:A:ARG:HG3	10	0.8
(1,494)	1:3:A:GLU:HB2	1:7:A:LEU:H	3	0.8
(1,434)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	6	0.8
(1,355)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	7	0.8
(1,355)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	7	0.8
(1,353)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	5	0.8
(1,353)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	5	0.8
(1,275)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	1	0.8
(1,275)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	7	0.8
(1,275)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	10	0.8
(1,240)	1:21:A:ARG:H	1:21:A:ARG:HG3	10	0.8
(3,57)	1:3:A:GLU:HB2	1:7:A:LEU:H	7	0.79
(2,390)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	2	0.79
(2,214)	1:21:A:ARG:H	1:21:A:ARG:HG3	7	0.79
(1,494)	1:3:A:GLU:HB2	1:7:A:LEU:H	7	0.79
(1,434)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	2	0.79
(1,240)	1:21:A:ARG:H	1:21:A:ARG:HG3	7	0.79
(3,50)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	7	0.78
(3,42)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	6	0.78
(2,390)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	1	0.78
(2,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	2	0.78
(2,214)	1:21:A:ARG:H	1:21:A:ARG:HG3	1	0.78
(2,214)	1:21:A:ARG:H	1:21:A:ARG:HG3	5	0.78
(1,460)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	7	0.78
(1,434)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	1	0.78
(1,386)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	6	0.78
(1,275)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	2	0.78
(1,240)	1:21:A:ARG:H	1:21:A:ARG:HG3	1	0.78
(1,240)	1:21:A:ARG:H	1:21:A:ARG:HG3	5	0.78
(3,57)	1:3:A:GLU:HB2	1:7:A:LEU:H	1	0.77
(3,57)	1:3:A:GLU:HB2	1:7:A:LEU:H	8	0.77
(3,57)	1:3:A:GLU:HB2	1:7:A:LEU:H	10	0.77
(3,50)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	1	0.77
(3,50)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	2	0.77
(3,50)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	3	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,50)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	4	0.77
(3,50)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	5	0.77
(3,50)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	6	0.77
(3,50)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	8	0.77
(3,50)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	9	0.77
(3,50)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.77
(3,42)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	3	0.77
(3,42)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	8	0.77
(3,4)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.77
(2,655)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	1	0.77
(2,655)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	1	0.77
(2,655)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	1	0.77
(2,655)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	6	0.77
(2,655)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	6	0.77
(2,655)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	6	0.77
(2,390)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	8	0.77
(2,390)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	9	0.77
(2,318)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	5	0.77
(2,318)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	5	0.77
(1,733)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	1	0.77
(1,733)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	1	0.77
(1,733)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	1	0.77
(1,733)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	6	0.77
(1,733)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	6	0.77
(1,733)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	6	0.77
(1,494)	1:3:A:GLU:HB2	1:7:A:LEU:H	1	0.77
(1,494)	1:3:A:GLU:HB2	1:7:A:LEU:H	8	0.77
(1,494)	1:3:A:GLU:HB2	1:7:A:LEU:H	10	0.77
(1,460)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	1	0.77
(1,460)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	2	0.77
(1,460)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	3	0.77
(1,460)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	4	0.77
(1,460)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	5	0.77
(1,460)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	6	0.77
(1,460)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	8	0.77
(1,460)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	9	0.77
(1,460)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.77
(1,434)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	8	0.77
(1,434)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	9	0.77
(1,386)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	3	0.77
(1,386)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	8	0.77
(1,355)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	5	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	5	0.77
(1,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.77
(3,57)	1:3:A:GLU:HB2	1:7:A:LEU:H	2	0.76
(3,57)	1:3:A:GLU:HB2	1:7:A:LEU:H	6	0.76
(3,42)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	4	0.76
(1,494)	1:3:A:GLU:HB2	1:7:A:LEU:H	2	0.76
(1,494)	1:3:A:GLU:HB2	1:7:A:LEU:H	6	0.76
(1,386)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	4	0.76
(3,57)	1:3:A:GLU:HB2	1:7:A:LEU:H	9	0.75
(3,42)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	7	0.75
(3,42)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	9	0.75
(2,390)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	3	0.75
(2,318)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	3	0.75
(2,318)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	3	0.75
(1,494)	1:3:A:GLU:HB2	1:7:A:LEU:H	9	0.75
(1,434)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	3	0.75
(1,386)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	7	0.75
(1,386)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	9	0.75
(1,355)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	3	0.75
(1,355)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	3	0.75
(3,57)	1:3:A:GLU:HB2	1:7:A:LEU:H	5	0.74
(3,42)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	2	0.74
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.74
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.74
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.74
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.74
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.74
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.74
(2,318)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	6	0.74
(2,318)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	6	0.74
(1,494)	1:3:A:GLU:HB2	1:7:A:LEU:H	5	0.74
(1,386)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	2	0.74
(1,355)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	6	0.74
(1,355)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	6	0.74
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.74
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.74
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.74
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.74
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.74
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.74
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.73
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.73
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.73
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.73
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.73
(2,390)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	4	0.73
(2,390)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	5	0.73
(1,434)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	4	0.73
(1,434)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	5	0.73
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.73
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.73
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.73
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.73
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.73
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.73
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.72
(3,10)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.72
(2,318)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	8	0.72
(2,318)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	8	0.72
(1,355)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	8	0.72
(1,355)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	8	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.72
(1,70)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.72
(3,4)	1:3:A:GLU:H	1:3:A:GLU:HG3	6	0.71
(2,318)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	0.71
(2,318)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	0.71
(1,355)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	0.71
(1,355)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	0.71
(1,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	6	0.71
(3,42)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	10	0.7
(1,386)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	10	0.7
(3,64)	1:21:A:ARG:H	1:22:A:PRO:HD2	3	0.69
(3,64)	1:21:A:ARG:H	1:22:A:PRO:HD2	4	0.69
(3,64)	1:21:A:ARG:H	1:22:A:PRO:HD2	6	0.69
(3,64)	1:21:A:ARG:H	1:22:A:PRO:HD2	9	0.69
(2,318)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	2	0.69
(2,318)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	2	0.69
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.69
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.69
(1,532)	1:21:A:ARG:H	1:22:A:PRO:HD2	3	0.69
(1,532)	1:21:A:ARG:H	1:22:A:PRO:HD2	4	0.69
(1,532)	1:21:A:ARG:H	1:22:A:PRO:HD2	6	0.69
(1,532)	1:21:A:ARG:H	1:22:A:PRO:HD2	9	0.69
(1,355)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	2	0.69
(1,355)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	2	0.69
(1,55)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.69
(1,55)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.69
(3,64)	1:21:A:ARG:H	1:22:A:PRO:HD2	8	0.68
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	1	0.68
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	2	0.68
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.68
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.68
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:21:A:ARG:H	1:22:A:PRO:HD2	8	0.68
(1,55)	1:6:A:ARG:H	1:6:A:ARG:HB3	1	0.68
(1,55)	1:6:A:ARG:H	1:6:A:ARG:HB3	2	0.68
(1,55)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.68
(1,55)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.68
(1,55)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.68
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	7	0.67
(1,55)	1:6:A:ARG:H	1:6:A:ARG:HB3	7	0.67
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.66
(3,6)	1:5:A:VAL:H	1:5:A:VAL:HB	10	0.66
(2,529)	1:5:A:VAL:H	1:6:A:ARG:HB3	8	0.66
(1,601)	1:5:A:VAL:H	1:6:A:ARG:HB3	8	0.66
(1,128)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.66
(1,30)	1:5:A:VAL:H	1:5:A:VAL:HB	10	0.66
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG3	5	0.65
(2,655)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	2	0.65
(2,655)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	2	0.65
(2,655)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	2	0.65
(2,529)	1:5:A:VAL:H	1:6:A:ARG:HB3	3	0.65
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.65
(1,733)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	2	0.65
(1,733)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	2	0.65
(1,733)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	2	0.65
(1,601)	1:5:A:VAL:H	1:6:A:ARG:HB3	3	0.65
(1,128)	1:10:A:GLN:H	1:10:A:GLN:HG3	5	0.65
(1,55)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.65
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG3	4	0.64
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG3	7	0.64
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.64
(1,128)	1:10:A:GLN:H	1:10:A:GLN:HG3	4	0.64
(1,128)	1:10:A:GLN:H	1:10:A:GLN:HG3	7	0.64
(1,55)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.64
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG3	9	0.63
(3,6)	1:5:A:VAL:H	1:5:A:VAL:HB	1	0.63
(3,6)	1:5:A:VAL:H	1:5:A:VAL:HB	2	0.63
(3,6)	1:5:A:VAL:H	1:5:A:VAL:HB	5	0.63
(2,655)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	3	0.63
(2,655)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	3	0.63
(2,655)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	3	0.63
(2,655)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	8	0.63
(2,655)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	8	0.63
(2,655)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	8	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,507)	1:23:A:PRO:HB3	1:25:A:SER:H	1	0.63
(2,367)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	6	0.63
(2,325)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	5	0.63
(2,318)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.63
(2,318)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.63
(2,231)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	3	0.63
(2,231)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	4	0.63
(2,231)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	6	0.63
(1,733)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	3	0.63
(1,733)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	3	0.63
(1,733)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	3	0.63
(1,733)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	8	0.63
(1,733)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	8	0.63
(1,733)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	8	0.63
(1,577)	1:23:A:PRO:HB3	1:25:A:SER:H	1	0.63
(1,410)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	6	0.63
(1,365)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	5	0.63
(1,355)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.63
(1,355)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.63
(1,257)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	3	0.63
(1,257)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	4	0.63
(1,257)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	6	0.63
(1,128)	1:10:A:GLN:H	1:10:A:GLN:HG3	9	0.63
(1,30)	1:5:A:VAL:H	1:5:A:VAL:HB	1	0.63
(1,30)	1:5:A:VAL:H	1:5:A:VAL:HB	2	0.63
(1,30)	1:5:A:VAL:H	1:5:A:VAL:HB	5	0.63
(3,71)	1:24:A:PRO:HB3	1:25:A:SER:H	1	0.62
(3,57)	1:3:A:GLU:HB2	1:7:A:LEU:H	4	0.62
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.62
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.62
(2,529)	1:5:A:VAL:H	1:6:A:ARG:HB3	7	0.62
(2,367)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.62
(2,250)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	3	0.62
(2,250)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	4	0.62
(2,250)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	6	0.62
(2,250)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	8	0.62
(2,250)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	9	0.62
(2,231)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	7	0.62
(2,231)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	8	0.62
(2,231)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	9	0.62
(2,231)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	10	0.62
(1,601)	1:5:A:VAL:H	1:6:A:ARG:HB3	7	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:24:A:PRO:HB3	1:25:A:SER:H	1	0.62
(1,494)	1:3:A:GLU:HB2	1:7:A:LEU:H	4	0.62
(1,410)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.62
(1,278)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	3	0.62
(1,278)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	4	0.62
(1,278)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	6	0.62
(1,278)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	8	0.62
(1,278)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	9	0.62
(1,257)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	7	0.62
(1,257)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	8	0.62
(1,257)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	9	0.62
(1,257)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	10	0.62
(1,128)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.62
(1,128)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.62
(3,82)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.61
(3,37)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	7	0.61
(3,37)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	7	0.61
(3,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	1	0.61
(3,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	1	0.61
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG3	1	0.61
(2,367)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	7	0.61
(2,231)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	1	0.61
(1,781)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.61
(1,410)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	7	0.61
(1,353)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	7	0.61
(1,353)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	7	0.61
(1,350)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	1	0.61
(1,350)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	1	0.61
(1,257)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	1	0.61
(1,128)	1:10:A:GLN:H	1:10:A:GLN:HG3	1	0.61
(3,82)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.6
(3,82)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.6
(3,82)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.6
(3,82)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.6
(3,82)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.6
(3,82)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.6
(3,82)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.6
(3,82)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.6
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.6
(2,367)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	9	0.6
(2,318)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	4	0.6
(2,318)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	4	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,231)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	2	0.6
(2,231)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	5	0.6
(2,214)	1:21:A:ARG:H	1:21:A:ARG:HG3	2	0.6
(1,781)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.6
(1,781)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.6
(1,781)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.6
(1,781)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.6
(1,781)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.6
(1,781)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.6
(1,781)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.6
(1,781)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.6
(1,410)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	9	0.6
(1,355)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	4	0.6
(1,355)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	4	0.6
(1,257)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	2	0.6
(1,257)	1:21:A:ARG:HB2	1:21:A:ARG:HG2	5	0.6
(1,240)	1:21:A:ARG:H	1:21:A:ARG:HG3	2	0.6
(1,128)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.6
(3,82)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.59
(3,71)	1:24:A:PRO:HB3	1:25:A:SER:H	9	0.59
(2,655)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	5	0.59
(2,655)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	5	0.59
(2,655)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	5	0.59
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	4	0.59
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	4	0.59
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	4	0.59
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	6	0.59
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	6	0.59
(2,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	10	0.59
(2,318)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	1	0.59
(2,318)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	1	0.59
(1,781)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.59
(1,733)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	5	0.59
(1,733)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	5	0.59
(1,733)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	5	0.59
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	4	0.59
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	4	0.59
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	4	0.59
(1,579)	1:24:A:PRO:HB3	1:25:A:SER:H	9	0.59
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	6	0.59
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	6	0.59
(1,406)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	10	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	1	0.59
(1,355)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	1	0.59
(3,63)	1:7:A:LEU:HG	1:8:A:TYR:H	7	0.58
(3,63)	1:7:A:LEU:HG	1:8:A:TYR:H	9	0.58
(3,4)	1:3:A:GLU:H	1:3:A:GLU:HG3	5	0.58
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	10	0.58
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	10	0.58
(2,367)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	3	0.58
(2,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	1	0.58
(2,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	3	0.58
(2,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	4	0.58
(2,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	6	0.58
(2,325)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	1	0.58
(2,325)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	9	0.58
(2,325)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	10	0.58
(1,522)	1:7:A:LEU:HG	1:8:A:TYR:H	7	0.58
(1,522)	1:7:A:LEU:HG	1:8:A:TYR:H	9	0.58
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	10	0.58
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	10	0.58
(1,410)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	3	0.58
(1,406)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	1	0.58
(1,406)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	3	0.58
(1,406)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	4	0.58
(1,406)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	6	0.58
(1,365)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	1	0.58
(1,365)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	9	0.58
(1,365)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	10	0.58
(1,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	5	0.58
(3,74)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	6	0.57
(3,74)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	8	0.57
(3,74)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	9	0.57
(3,71)	1:24:A:PRO:HB3	1:25:A:SER:H	2	0.57
(3,71)	1:24:A:PRO:HB3	1:25:A:SER:H	5	0.57
(3,42)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	1	0.57
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.57
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.57
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.57
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.57
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD2	9	0.57
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD3	9	0.57
(2,655)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	10	0.57
(2,655)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,655)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	10	0.57
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	1	0.57
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	1	0.57
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	7	0.57
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	7	0.57
(2,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	2	0.57
(2,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	9	0.57
(2,325)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	3	0.57
(2,325)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	4	0.57
(2,325)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	7	0.57
(2,325)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	8	0.57
(2,92)	1:9:A:ILE:H	1:9:A:ILE:HG12	4	0.57
(1,733)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	10	0.57
(1,733)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	10	0.57
(1,733)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	10	0.57
(1,667)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	6	0.57
(1,667)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	8	0.57
(1,667)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	9	0.57
(1,579)	1:24:A:PRO:HB3	1:25:A:SER:H	2	0.57
(1,579)	1:24:A:PRO:HB3	1:25:A:SER:H	5	0.57
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	1	0.57
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	1	0.57
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	7	0.57
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	7	0.57
(1,406)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	2	0.57
(1,406)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	9	0.57
(1,386)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	1	0.57
(1,365)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	3	0.57
(1,365)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	4	0.57
(1,365)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	7	0.57
(1,365)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	8	0.57
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.57
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.57
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.57
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.57
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD2	9	0.57
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD3	9	0.57
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	4	0.57
(3,74)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	3	0.56
(3,74)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	4	0.56
(3,70)	1:9:A:ILE:HD11	1:10:A:GLN:H	2	0.56
(3,70)	1:9:A:ILE:HD12	1:10:A:GLN:H	2	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,70)	1:9:A:ILE:HD13	1:10:A:GLN:H	2	0.56
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.56
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.56
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.56
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.56
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.56
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.56
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.56
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.56
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.56
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.56
(3,37)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	3	0.56
(3,37)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	3	0.56
(3,20)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.56
(3,1)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	3	0.56
(3,1)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	7	0.56
(3,1)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	8	0.56
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	3	0.56
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	3	0.56
(2,367)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	1	0.56
(2,367)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	2	0.56
(2,367)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	4	0.56
(2,367)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	8	0.56
(2,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	7	0.56
(2,347)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	8	0.56
(2,325)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	2	0.56
(2,325)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	6	0.56
(2,233)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	3	0.56
(2,233)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	4	0.56
(2,233)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	6	0.56
(2,233)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	9	0.56
(2,92)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.56
(2,92)	1:9:A:ILE:H	1:9:A:ILE:HG12	3	0.56
(2,92)	1:9:A:ILE:H	1:9:A:ILE:HG12	6	0.56
(2,92)	1:9:A:ILE:H	1:9:A:ILE:HG12	8	0.56
(1,667)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	3	0.56
(1,667)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	4	0.56
(1,576)	1:9:A:ILE:HD11	1:10:A:GLN:H	2	0.56
(1,576)	1:9:A:ILE:HD12	1:10:A:GLN:H	2	0.56
(1,576)	1:9:A:ILE:HD13	1:10:A:GLN:H	2	0.56
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	3	0.56
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	3	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	1	0.56
(1,410)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	2	0.56
(1,410)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	4	0.56
(1,410)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	8	0.56
(1,406)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	7	0.56
(1,389)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	8	0.56
(1,365)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	2	0.56
(1,365)	1:11:A:TRP:HE1	1:24:A:PRO:HD2	6	0.56
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.56
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.56
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.56
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.56
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.56
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.56
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.56
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.56
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.56
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.56
(1,353)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	3	0.56
(1,353)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	3	0.56
(1,260)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	3	0.56
(1,260)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	4	0.56
(1,260)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	6	0.56
(1,260)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	9	0.56
(1,128)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.56
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.56
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	3	0.56
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	6	0.56
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	8	0.56
(1,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	3	0.56
(1,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	7	0.56
(1,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	8	0.56
(3,37)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	2	0.55
(3,37)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	2	0.55
(3,37)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	6	0.55
(3,37)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	6	0.55
(3,37)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	9	0.55
(3,37)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	9	0.55
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD2	2	0.55
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD3	2	0.55
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD2	5	0.55
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD3	5	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD2	7	0.55
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD3	7	0.55
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD2	8	0.55
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD3	8	0.55
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD2	10	0.55
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD3	10	0.55
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	2	0.55
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	2	0.55
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	2	0.55
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.55
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.55
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.55
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.55
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.55
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.55
(3,1)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	1	0.55
(3,1)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	10	0.55
(2,655)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	9	0.55
(2,655)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	9	0.55
(2,655)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	9	0.55
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	4	0.55
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	4	0.55
(2,347)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	1	0.55
(2,347)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	3	0.55
(2,347)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	6	0.55
(2,233)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	7	0.55
(2,233)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	8	0.55
(2,233)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.55
(2,92)	1:9:A:ILE:H	1:9:A:ILE:HG12	9	0.55
(2,92)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.55
(1,733)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	9	0.55
(1,733)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	9	0.55
(1,733)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	9	0.55
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	4	0.55
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	4	0.55
(1,389)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	1	0.55
(1,389)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	3	0.55
(1,389)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	6	0.55
(1,353)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	2	0.55
(1,353)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	2	0.55
(1,353)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	6	0.55
(1,353)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	9	0.55
(1,353)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	9	0.55
(1,260)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	7	0.55
(1,260)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	8	0.55
(1,260)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.55
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD2	2	0.55
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD3	2	0.55
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD2	5	0.55
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD3	5	0.55
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD2	7	0.55
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD3	7	0.55
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD2	8	0.55
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD3	8	0.55
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD2	10	0.55
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD3	10	0.55
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	9	0.55
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.55
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	2	0.55
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	2	0.55
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	2	0.55
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.55
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.55
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.55
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.55
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.55
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.55
(1,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	1	0.55
(1,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	10	0.55
(3,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	4	0.54
(3,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	4	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	9	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	9	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	9	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.54
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.54
(3,6)	1:5:A:VAL:H	1:5:A:VAL:HB	9	0.54
(3,1)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	2	0.54
(3,1)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	5	0.54
(3,1)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	9	0.54
(2,655)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	7	0.54
(2,655)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	7	0.54
(2,655)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	7	0.54
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	5	0.54
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	5	0.54
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	8	0.54
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	8	0.54
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	9	0.54
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	9	0.54
(2,347)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	4	0.54
(2,347)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	5	0.54
(2,347)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	9	0.54
(2,347)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	10	0.54
(2,233)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	1	0.54
(2,233)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	5	0.54
(2,92)	1:9:A:ILE:H	1:9:A:ILE:HG12	2	0.54
(2,92)	1:9:A:ILE:H	1:9:A:ILE:HG12	5	0.54
(2,92)	1:9:A:ILE:H	1:9:A:ILE:HG12	7	0.54
(1,733)	1:9:A:ILE:HG21	1:13:A:LYS:HG2	7	0.54
(1,733)	1:9:A:ILE:HG22	1:13:A:LYS:HG2	7	0.54
(1,733)	1:9:A:ILE:HG23	1:13:A:LYS:HG2	7	0.54
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	5	0.54
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	5	0.54
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	8	0.54
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	8	0.54
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	9	0.54
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	9	0.54
(1,389)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	4	0.54
(1,389)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	5	0.54
(1,389)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	9	0.54
(1,389)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	10	0.54
(1,350)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	4	0.54
(1,350)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	4	0.54
(1,260)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	1	0.54
(1,260)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	5	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	2	0.54
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	5	0.54
(1,107)	1:9:A:ILE:H	1:9:A:ILE:HG12	7	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	9	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	9	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	9	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.54
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.54
(1,30)	1:5:A:VAL:H	1:5:A:VAL:HB	9	0.54
(1,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	2	0.54
(1,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	5	0.54
(1,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	9	0.54
(3,37)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	8	0.53
(3,37)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	8	0.53
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD2	1	0.53
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD3	1	0.53
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD2	6	0.53
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD3	6	0.53
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	7	0.53
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	7	0.53
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	7	0.53
(3,1)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	6	0.53
(2,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	5	0.53
(2,347)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	7	0.53
(1,406)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	5	0.53
(1,389)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	7	0.53
(1,353)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	8	0.53
(1,353)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	8	0.53
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD2	1	0.53
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD3	1	0.53
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD2	6	0.53
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD3	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	7	0.53
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	7	0.53
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	7	0.53
(1,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	6	0.53
(3,30)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	10	0.52
(3,30)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	10	0.52
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD2	3	0.52
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD3	3	0.52
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD2	4	0.52
(3,23)	1:13:A:LYS:HA	1:13:A:LYS:HD3	4	0.52
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.52
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.52
(3,12)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.52
(2,347)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	2	0.52
(2,233)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	2	0.52
(1,389)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	2	0.52
(1,320)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	10	0.52
(1,320)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	10	0.52
(1,260)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	2	0.52
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD2	3	0.52
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD3	3	0.52
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD2	4	0.52
(1,168)	1:13:A:LYS:HA	1:13:A:LYS:HD3	4	0.52
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.52
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.52
(1,79)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.52
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.51
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.51
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.51
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.51
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.51
(3,38)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.51
(3,30)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	6	0.51
(3,30)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	6	0.51
(2,367)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	5	0.51
(2,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.51
(2,160)	1:13:A:LYS:H	1:13:A:LYS:HG2	4	0.51
(2,160)	1:13:A:LYS:H	1:13:A:LYS:HG2	6	0.51
(1,410)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	5	0.51
(1,406)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.51
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.51
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.51
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.51
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.51
(1,356)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.51
(1,320)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	6	0.51
(1,320)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	6	0.51
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	4	0.51
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	6	0.51
(3,71)	1:24:A:PRO:HB3	1:25:A:SER:H	3	0.5
(3,71)	1:24:A:PRO:HB3	1:25:A:SER:H	8	0.5
(3,63)	1:7:A:LEU:HG	1:8:A:TYR:H	1	0.5
(3,63)	1:7:A:LEU:HG	1:8:A:TYR:H	2	0.5
(3,63)	1:7:A:LEU:HG	1:8:A:TYR:H	6	0.5
(3,63)	1:7:A:LEU:HG	1:8:A:TYR:H	8	0.5
(3,30)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	2	0.5
(3,30)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	2	0.5
(3,18)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	6	0.5
(3,6)	1:5:A:VAL:H	1:5:A:VAL:HB	4	0.5
(1,579)	1:24:A:PRO:HB3	1:25:A:SER:H	3	0.5
(1,579)	1:24:A:PRO:HB3	1:25:A:SER:H	8	0.5
(1,522)	1:7:A:LEU:HG	1:8:A:TYR:H	1	0.5
(1,522)	1:7:A:LEU:HG	1:8:A:TYR:H	2	0.5
(1,522)	1:7:A:LEU:HG	1:8:A:TYR:H	6	0.5
(1,522)	1:7:A:LEU:HG	1:8:A:TYR:H	8	0.5
(1,320)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	2	0.5
(1,320)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	2	0.5
(1,124)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	6	0.5
(1,30)	1:5:A:VAL:H	1:5:A:VAL:HB	4	0.5
(3,70)	1:9:A:ILE:HD11	1:10:A:GLN:H	1	0.49
(3,70)	1:9:A:ILE:HD12	1:10:A:GLN:H	1	0.49
(3,70)	1:9:A:ILE:HD13	1:10:A:GLN:H	1	0.49
(3,70)	1:9:A:ILE:HD11	1:10:A:GLN:H	7	0.49
(3,70)	1:9:A:ILE:HD12	1:10:A:GLN:H	7	0.49
(3,70)	1:9:A:ILE:HD13	1:10:A:GLN:H	7	0.49
(3,70)	1:9:A:ILE:HD11	1:10:A:GLN:H	8	0.49
(3,70)	1:9:A:ILE:HD12	1:10:A:GLN:H	8	0.49
(3,70)	1:9:A:ILE:HD13	1:10:A:GLN:H	8	0.49
(3,70)	1:9:A:ILE:HD11	1:10:A:GLN:H	9	0.49
(3,70)	1:9:A:ILE:HD12	1:10:A:GLN:H	9	0.49
(3,70)	1:9:A:ILE:HD13	1:10:A:GLN:H	9	0.49
(3,63)	1:7:A:LEU:HG	1:8:A:TYR:H	3	0.49
(3,63)	1:7:A:LEU:HG	1:8:A:TYR:H	10	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	0.49
(3,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	0.49
(3,18)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	1	0.49
(3,18)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	2	0.49
(3,18)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	3	0.49
(3,18)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	4	0.49
(3,18)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	5	0.49
(3,18)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	7	0.49
(3,18)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	8	0.49
(3,18)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	9	0.49
(3,18)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	10	0.49
(3,6)	1:5:A:VAL:H	1:5:A:VAL:HB	8	0.49
(3,4)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.49
(2,529)	1:5:A:VAL:H	1:6:A:ARG:HB3	6	0.49
(2,160)	1:13:A:LYS:H	1:13:A:LYS:HG2	1	0.49
(2,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	4	0.49
(1,601)	1:5:A:VAL:H	1:6:A:ARG:HB3	6	0.49
(1,576)	1:9:A:ILE:HD11	1:10:A:GLN:H	1	0.49
(1,576)	1:9:A:ILE:HD12	1:10:A:GLN:H	1	0.49
(1,576)	1:9:A:ILE:HD13	1:10:A:GLN:H	1	0.49
(1,576)	1:9:A:ILE:HD11	1:10:A:GLN:H	7	0.49
(1,576)	1:9:A:ILE:HD12	1:10:A:GLN:H	7	0.49
(1,576)	1:9:A:ILE:HD13	1:10:A:GLN:H	7	0.49
(1,576)	1:9:A:ILE:HD11	1:10:A:GLN:H	8	0.49
(1,576)	1:9:A:ILE:HD12	1:10:A:GLN:H	8	0.49
(1,576)	1:9:A:ILE:HD13	1:10:A:GLN:H	8	0.49
(1,576)	1:9:A:ILE:HD11	1:10:A:GLN:H	9	0.49
(1,576)	1:9:A:ILE:HD12	1:10:A:GLN:H	9	0.49
(1,576)	1:9:A:ILE:HD13	1:10:A:GLN:H	9	0.49
(1,522)	1:7:A:LEU:HG	1:8:A:TYR:H	3	0.49
(1,522)	1:7:A:LEU:HG	1:8:A:TYR:H	10	0.49
(1,350)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	10	0.49
(1,350)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	10	0.49
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	1	0.49
(1,124)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	1	0.49
(1,124)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	2	0.49
(1,124)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	3	0.49
(1,124)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	4	0.49
(1,124)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	5	0.49
(1,124)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	7	0.49
(1,124)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	8	0.49
(1,124)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	9	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	10	0.49
(1,30)	1:5:A:VAL:H	1:5:A:VAL:HB	8	0.49
(1,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.49
(1,12)	1:3:A:GLU:HB2	1:3:A:GLU:HG3	4	0.49
(3,71)	1:24:A:PRO:HB3	1:25:A:SER:H	4	0.48
(3,70)	1:9:A:ILE:HD11	1:10:A:GLN:H	3	0.48
(3,70)	1:9:A:ILE:HD12	1:10:A:GLN:H	3	0.48
(3,70)	1:9:A:ILE:HD13	1:10:A:GLN:H	3	0.48
(3,70)	1:9:A:ILE:HD11	1:10:A:GLN:H	6	0.48
(3,70)	1:9:A:ILE:HD12	1:10:A:GLN:H	6	0.48
(3,70)	1:9:A:ILE:HD13	1:10:A:GLN:H	6	0.48
(3,63)	1:7:A:LEU:HG	1:8:A:TYR:H	5	0.48
(3,42)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	5	0.48
(3,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	3	0.48
(3,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	3	0.48
(1,579)	1:24:A:PRO:HB3	1:25:A:SER:H	4	0.48
(1,576)	1:9:A:ILE:HD11	1:10:A:GLN:H	3	0.48
(1,576)	1:9:A:ILE:HD12	1:10:A:GLN:H	3	0.48
(1,576)	1:9:A:ILE:HD13	1:10:A:GLN:H	3	0.48
(1,576)	1:9:A:ILE:HD11	1:10:A:GLN:H	6	0.48
(1,576)	1:9:A:ILE:HD12	1:10:A:GLN:H	6	0.48
(1,576)	1:9:A:ILE:HD13	1:10:A:GLN:H	6	0.48
(1,522)	1:7:A:LEU:HG	1:8:A:TYR:H	5	0.48
(1,386)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	5	0.48
(1,350)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	3	0.48
(1,350)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	3	0.48
(3,70)	1:9:A:ILE:HD11	1:10:A:GLN:H	4	0.47
(3,70)	1:9:A:ILE:HD12	1:10:A:GLN:H	4	0.47
(3,70)	1:9:A:ILE:HD13	1:10:A:GLN:H	4	0.47
(3,70)	1:9:A:ILE:HD11	1:10:A:GLN:H	5	0.47
(3,70)	1:9:A:ILE:HD12	1:10:A:GLN:H	5	0.47
(3,70)	1:9:A:ILE:HD13	1:10:A:GLN:H	5	0.47
(3,70)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.47
(3,70)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.47
(3,70)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.47
(3,37)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	10	0.47
(3,37)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	10	0.47
(3,6)	1:5:A:VAL:H	1:5:A:VAL:HB	3	0.47
(3,6)	1:5:A:VAL:H	1:5:A:VAL:HB	7	0.47
(3,4)	1:3:A:GLU:H	1:3:A:GLU:HG3	2	0.47
(1,576)	1:9:A:ILE:HD11	1:10:A:GLN:H	4	0.47
(1,576)	1:9:A:ILE:HD12	1:10:A:GLN:H	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,576)	1:9:A:ILE:HD13	1:10:A:GLN:H	4	0.47
(1,576)	1:9:A:ILE:HD11	1:10:A:GLN:H	5	0.47
(1,576)	1:9:A:ILE:HD12	1:10:A:GLN:H	5	0.47
(1,576)	1:9:A:ILE:HD13	1:10:A:GLN:H	5	0.47
(1,576)	1:9:A:ILE:HD11	1:10:A:GLN:H	10	0.47
(1,576)	1:9:A:ILE:HD12	1:10:A:GLN:H	10	0.47
(1,576)	1:9:A:ILE:HD13	1:10:A:GLN:H	10	0.47
(1,353)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	10	0.47
(1,353)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	10	0.47
(1,30)	1:5:A:VAL:H	1:5:A:VAL:HB	3	0.47
(1,30)	1:5:A:VAL:H	1:5:A:VAL:HB	7	0.47
(1,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	2	0.47
(3,72)	1:3:A:GLU:HG2	1:5:A:VAL:H	1	0.46
(3,71)	1:24:A:PRO:HB3	1:25:A:SER:H	10	0.46
(3,63)	1:7:A:LEU:HG	1:8:A:TYR:H	4	0.46
(3,62)	1:12:A:LEU:HD21	1:13:A:LYS:H	1	0.46
(3,62)	1:12:A:LEU:HD22	1:13:A:LYS:H	1	0.46
(3,62)	1:12:A:LEU:HD23	1:13:A:LYS:H	1	0.46
(3,62)	1:12:A:LEU:HD21	1:13:A:LYS:H	3	0.46
(3,62)	1:12:A:LEU:HD22	1:13:A:LYS:H	3	0.46
(3,62)	1:12:A:LEU:HD23	1:13:A:LYS:H	3	0.46
(3,62)	1:12:A:LEU:HD21	1:13:A:LYS:H	9	0.46
(3,62)	1:12:A:LEU:HD22	1:13:A:LYS:H	9	0.46
(3,62)	1:12:A:LEU:HD23	1:13:A:LYS:H	9	0.46
(3,37)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	1	0.46
(3,37)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	1	0.46
(3,33)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	0.46
(3,33)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	0.46
(3,33)	1:8:A:TYR:HD1	1:12:A:LEU:HG	9	0.46
(3,33)	1:8:A:TYR:HD2	1:12:A:LEU:HG	9	0.46
(3,30)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	1	0.46
(3,30)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	1	0.46
(3,30)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	4	0.46
(3,30)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	4	0.46
(3,6)	1:5:A:VAL:H	1:5:A:VAL:HB	6	0.46
(3,4)	1:3:A:GLU:H	1:3:A:GLU:HG3	3	0.46
(2,529)	1:5:A:VAL:H	1:6:A:ARG:HB3	4	0.46
(2,529)	1:5:A:VAL:H	1:6:A:ARG:HB3	5	0.46
(1,601)	1:5:A:VAL:H	1:6:A:ARG:HB3	4	0.46
(1,601)	1:5:A:VAL:H	1:6:A:ARG:HB3	5	0.46
(1,599)	1:3:A:GLU:HG2	1:5:A:VAL:H	1	0.46
(1,579)	1:24:A:PRO:HB3	1:25:A:SER:H	10	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:7:A:LEU:HG	1:8:A:TYR:H	4	0.46
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:H	1	0.46
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:H	1	0.46
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:H	1	0.46
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:H	3	0.46
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:H	3	0.46
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:H	3	0.46
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:H	9	0.46
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:H	9	0.46
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:H	9	0.46
(1,353)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	1	0.46
(1,353)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	1	0.46
(1,337)	1:8:A:TYR:HD1	1:12:A:LEU:HG	8	0.46
(1,337)	1:8:A:TYR:HD2	1:12:A:LEU:HG	8	0.46
(1,337)	1:8:A:TYR:HD1	1:12:A:LEU:HG	9	0.46
(1,337)	1:8:A:TYR:HD2	1:12:A:LEU:HG	9	0.46
(1,320)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	1	0.46
(1,320)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	1	0.46
(1,320)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	4	0.46
(1,320)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	4	0.46
(1,30)	1:5:A:VAL:H	1:5:A:VAL:HB	6	0.46
(1,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	3	0.46
(3,74)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	1	0.45
(3,74)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	5	0.45
(3,72)	1:3:A:GLU:HG2	1:5:A:VAL:H	10	0.45
(3,71)	1:24:A:PRO:HB3	1:25:A:SER:H	6	0.45
(3,71)	1:24:A:PRO:HB3	1:25:A:SER:H	7	0.45
(3,62)	1:12:A:LEU:HD21	1:13:A:LYS:H	4	0.45
(3,62)	1:12:A:LEU:HD22	1:13:A:LYS:H	4	0.45
(3,62)	1:12:A:LEU:HD23	1:13:A:LYS:H	4	0.45
(3,62)	1:12:A:LEU:HD21	1:13:A:LYS:H	5	0.45
(3,62)	1:12:A:LEU:HD22	1:13:A:LYS:H	5	0.45
(3,62)	1:12:A:LEU:HD23	1:13:A:LYS:H	5	0.45
(3,62)	1:12:A:LEU:HD21	1:13:A:LYS:H	7	0.45
(3,62)	1:12:A:LEU:HD22	1:13:A:LYS:H	7	0.45
(3,62)	1:12:A:LEU:HD23	1:13:A:LYS:H	7	0.45
(3,62)	1:12:A:LEU:HD21	1:13:A:LYS:H	8	0.45
(3,62)	1:12:A:LEU:HD22	1:13:A:LYS:H	8	0.45
(3,62)	1:12:A:LEU:HD23	1:13:A:LYS:H	8	0.45
(3,33)	1:8:A:TYR:HD1	1:12:A:LEU:HG	2	0.45
(3,33)	1:8:A:TYR:HD2	1:12:A:LEU:HG	2	0.45
(3,30)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,30)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	3	0.45
(3,30)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	8	0.45
(3,30)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	8	0.45
(3,26)	1:21:A:ARG:H	1:21:A:ARG:HG2	5	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD11	2	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD12	2	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD13	2	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD11	5	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD12	5	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD13	5	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD11	6	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD12	6	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD13	6	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD11	7	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD12	7	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD13	7	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.45
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.45
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	6	0.45
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	6	0.45
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	6	0.45
(3,4)	1:3:A:GLU:H	1:3:A:GLU:HG3	7	0.45
(1,667)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	1	0.45
(1,667)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	5	0.45
(1,599)	1:3:A:GLU:HG2	1:5:A:VAL:H	10	0.45
(1,579)	1:24:A:PRO:HB3	1:25:A:SER:H	6	0.45
(1,579)	1:24:A:PRO:HB3	1:25:A:SER:H	7	0.45
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:H	4	0.45
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:H	4	0.45
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:H	4	0.45
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:H	5	0.45
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:H	5	0.45
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:H	5	0.45
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:H	7	0.45
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:H	7	0.45
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:H	7	0.45
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:H	8	0.45
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:H	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:H	8	0.45
(1,337)	1:8:A:TYR:HD1	1:12:A:LEU:HG	2	0.45
(1,337)	1:8:A:TYR:HD2	1:12:A:LEU:HG	2	0.45
(1,320)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	3	0.45
(1,320)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	3	0.45
(1,320)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	8	0.45
(1,320)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	8	0.45
(1,239)	1:21:A:ARG:H	1:21:A:ARG:HG2	5	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD11	2	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD12	2	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD13	2	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD11	5	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD12	5	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD13	5	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD11	6	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD12	6	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD13	6	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD11	7	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD12	7	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD13	7	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.45
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.45
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG21	6	0.45
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG22	6	0.45
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG23	6	0.45
(1,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	7	0.45
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	1	0.44
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	1	0.44
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	1	0.44
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	4	0.44
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	4	0.44
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	4	0.44
(3,74)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	10	0.44
(3,69)	1:7:A:LEU:HB3	1:10:A:GLN:H	6	0.44
(3,69)	1:7:A:LEU:HB3	1:10:A:GLN:H	9	0.44
(3,62)	1:12:A:LEU:HD21	1:13:A:LYS:H	2	0.44
(3,62)	1:12:A:LEU:HD22	1:13:A:LYS:H	2	0.44
(3,62)	1:12:A:LEU:HD23	1:13:A:LYS:H	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,62)	1:12:A:LEU:HD21	1:13:A:LYS:H	6	0.44
(3,62)	1:12:A:LEU:HD22	1:13:A:LYS:H	6	0.44
(3,62)	1:12:A:LEU:HD23	1:13:A:LYS:H	6	0.44
(3,62)	1:12:A:LEU:HD21	1:13:A:LYS:H	10	0.44
(3,62)	1:12:A:LEU:HD22	1:13:A:LYS:H	10	0.44
(3,62)	1:12:A:LEU:HD23	1:13:A:LYS:H	10	0.44
(3,48)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	7	0.44
(3,48)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	7	0.44
(3,33)	1:8:A:TYR:HD1	1:12:A:LEU:HG	3	0.44
(3,33)	1:8:A:TYR:HD2	1:12:A:LEU:HG	3	0.44
(3,33)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	0.44
(3,33)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	0.44
(3,33)	1:8:A:TYR:HD1	1:12:A:LEU:HG	6	0.44
(3,33)	1:8:A:TYR:HD2	1:12:A:LEU:HG	6	0.44
(3,33)	1:8:A:TYR:HD1	1:12:A:LEU:HG	7	0.44
(3,33)	1:8:A:TYR:HD2	1:12:A:LEU:HG	7	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD11	1	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD12	1	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD13	1	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD11	3	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD12	3	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD13	3	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD11	8	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD12	8	0.44
(3,14)	1:9:A:ILE:HA	1:9:A:ILE:HD13	8	0.44
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	1	0.44
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	1	0.44
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	1	0.44
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	4	0.44
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	4	0.44
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	4	0.44
(1,667)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	10	0.44
(1,571)	1:7:A:LEU:HB3	1:10:A:GLN:H	6	0.44
(1,571)	1:7:A:LEU:HB3	1:10:A:GLN:H	9	0.44
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:H	2	0.44
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:H	2	0.44
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:H	2	0.44
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:H	6	0.44
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:H	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:H	6	0.44
(1,517)	1:12:A:LEU:HD21	1:13:A:LYS:H	10	0.44
(1,517)	1:12:A:LEU:HD22	1:13:A:LYS:H	10	0.44
(1,517)	1:12:A:LEU:HD23	1:13:A:LYS:H	10	0.44
(1,457)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	7	0.44
(1,457)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	7	0.44
(1,337)	1:8:A:TYR:HD1	1:12:A:LEU:HG	3	0.44
(1,337)	1:8:A:TYR:HD2	1:12:A:LEU:HG	3	0.44
(1,337)	1:8:A:TYR:HD1	1:12:A:LEU:HG	5	0.44
(1,337)	1:8:A:TYR:HD2	1:12:A:LEU:HG	5	0.44
(1,337)	1:8:A:TYR:HD1	1:12:A:LEU:HG	6	0.44
(1,337)	1:8:A:TYR:HD2	1:12:A:LEU:HG	6	0.44
(1,337)	1:8:A:TYR:HD1	1:12:A:LEU:HG	7	0.44
(1,337)	1:8:A:TYR:HD2	1:12:A:LEU:HG	7	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD11	1	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD12	1	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD13	1	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD11	3	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD12	3	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD13	3	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD11	8	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD12	8	0.44
(1,97)	1:9:A:ILE:HA	1:9:A:ILE:HD13	8	0.44
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	5	0.43
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	5	0.43
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	5	0.43
(3,74)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	7	0.43
(3,72)	1:3:A:GLU:HG2	1:5:A:VAL:H	2	0.43
(3,72)	1:3:A:GLU:HG2	1:5:A:VAL:H	5	0.43
(3,69)	1:7:A:LEU:HB3	1:10:A:GLN:H	1	0.43
(3,69)	1:7:A:LEU:HB3	1:10:A:GLN:H	7	0.43
(3,31)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	5	0.43
(3,31)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	5	0.43
(3,30)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	9	0.43
(3,30)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	9	0.43
(3,4)	1:3:A:GLU:H	1:3:A:GLU:HG3	1	0.43
(2,221)	1:21:A:ARG:HA	1:21:A:ARG:HG2	2	0.43
(2,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	1	0.43
(2,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	8	0.43
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	5	0.43
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	5	0.43
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	5	0.43
(1,667)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	7	0.43
(1,599)	1:3:A:GLU:HG2	1:5:A:VAL:H	2	0.43
(1,599)	1:3:A:GLU:HG2	1:5:A:VAL:H	5	0.43
(1,571)	1:7:A:LEU:HB3	1:10:A:GLN:H	1	0.43
(1,571)	1:7:A:LEU:HB3	1:10:A:GLN:H	7	0.43
(1,330)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	5	0.43
(1,330)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	5	0.43
(1,320)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	9	0.43
(1,320)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	9	0.43
(1,247)	1:21:A:ARG:HA	1:21:A:ARG:HG2	2	0.43
(1,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	1	0.43
(1,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	1	0.43
(1,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	6	0.43
(1,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	8	0.43
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	2	0.42
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	2	0.42
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	2	0.42
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	0.42
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	0.42
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	0.42
(3,72)	1:3:A:GLU:HG2	1:5:A:VAL:H	6	0.42
(3,69)	1:7:A:LEU:HB3	1:10:A:GLN:H	3	0.42
(3,69)	1:7:A:LEU:HB3	1:10:A:GLN:H	5	0.42
(3,69)	1:7:A:LEU:HB3	1:10:A:GLN:H	8	0.42
(3,69)	1:7:A:LEU:HB3	1:10:A:GLN:H	10	0.42
(3,48)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	2	0.42
(3,48)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	2	0.42
(3,48)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	3	0.42
(3,48)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	3	0.42
(3,48)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	5	0.42
(3,48)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	5	0.42
(3,48)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	8	0.42
(3,48)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	8	0.42
(3,31)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	3	0.42
(3,31)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	3	0.42
(3,31)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	6	0.42
(3,31)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	6	0.42
(3,31)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	7	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,31)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	7	0.42
(3,26)	1:21:A:ARG:H	1:21:A:ARG:HG2	1	0.42
(2,529)	1:5:A:VAL:H	1:6:A:ARG:HB3	1	0.42
(2,529)	1:5:A:VAL:H	1:6:A:ARG:HB3	9	0.42
(2,221)	1:21:A:ARG:HA	1:21:A:ARG:HG2	3	0.42
(2,221)	1:21:A:ARG:HA	1:21:A:ARG:HG2	6	0.42
(2,160)	1:13:A:LYS:H	1:13:A:LYS:HG2	2	0.42
(2,160)	1:13:A:LYS:H	1:13:A:LYS:HG2	8	0.42
(2,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	2	0.42
(2,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	4	0.42
(2,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	9	0.42
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	2	0.42
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	2	0.42
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	2	0.42
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	0.42
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	0.42
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	0.42
(1,601)	1:5:A:VAL:H	1:6:A:ARG:HB3	1	0.42
(1,601)	1:5:A:VAL:H	1:6:A:ARG:HB3	9	0.42
(1,599)	1:3:A:GLU:HG2	1:5:A:VAL:H	6	0.42
(1,571)	1:7:A:LEU:HB3	1:10:A:GLN:H	3	0.42
(1,571)	1:7:A:LEU:HB3	1:10:A:GLN:H	5	0.42
(1,571)	1:7:A:LEU:HB3	1:10:A:GLN:H	8	0.42
(1,571)	1:7:A:LEU:HB3	1:10:A:GLN:H	10	0.42
(1,457)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	2	0.42
(1,457)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	2	0.42
(1,457)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	3	0.42
(1,457)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	3	0.42
(1,457)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	5	0.42
(1,457)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	5	0.42
(1,457)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	8	0.42
(1,457)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	8	0.42
(1,330)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	3	0.42
(1,330)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	3	0.42
(1,330)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	6	0.42
(1,330)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	6	0.42
(1,330)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	7	0.42
(1,330)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	7	0.42
(1,247)	1:21:A:ARG:HA	1:21:A:ARG:HG2	3	0.42
(1,247)	1:21:A:ARG:HA	1:21:A:ARG:HG2	6	0.42
(1,239)	1:21:A:ARG:H	1:21:A:ARG:HG2	1	0.42
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	8	0.42
(1,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	2	0.42
(1,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	4	0.42
(1,5)	1:2:A:GLU:HB2	1:2:A:GLU:HG3	9	0.42
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	3	0.41
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	3	0.41
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	3	0.41
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	7	0.41
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	7	0.41
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	7	0.41
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	8	0.41
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	8	0.41
(3,75)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	8	0.41
(3,43)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	0.41
(3,37)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	4	0.41
(3,37)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	4	0.41
(3,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	2	0.41
(3,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	2	0.41
(3,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	9	0.41
(3,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	9	0.41
(3,35)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	5	0.41
(3,35)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	6	0.41
(3,35)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	7	0.41
(3,35)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	9	0.41
(3,35)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	10	0.41
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	3	0.41
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	3	0.41
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	3	0.41
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	7	0.41
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	7	0.41
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	7	0.41
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	9	0.41
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	9	0.41
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	9	0.41
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG11	4	0.41
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG12	4	0.41
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG13	4	0.41
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG11	6	0.41
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG12	6	0.41
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG13	6	0.41
(3,2)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	9	0.41
(2,221)	1:21:A:ARG:HA	1:21:A:ARG:HG2	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,221)	1:21:A:ARG:HA	1:21:A:ARG:HG2	8	0.41
(2,221)	1:21:A:ARG:HA	1:21:A:ARG:HG2	9	0.41
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	3	0.41
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	3	0.41
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	3	0.41
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	7	0.41
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	7	0.41
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	7	0.41
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	8	0.41
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	8	0.41
(1,698)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	8	0.41
(1,396)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	0.41
(1,353)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	4	0.41
(1,353)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	4	0.41
(1,350)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	2	0.41
(1,350)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	2	0.41
(1,350)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	9	0.41
(1,350)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	9	0.41
(1,342)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	5	0.41
(1,342)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	6	0.41
(1,342)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	7	0.41
(1,342)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	9	0.41
(1,342)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	10	0.41
(1,247)	1:21:A:ARG:HA	1:21:A:ARG:HG2	4	0.41
(1,247)	1:21:A:ARG:HA	1:21:A:ARG:HG2	8	0.41
(1,247)	1:21:A:ARG:HA	1:21:A:ARG:HG2	9	0.41
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG21	3	0.41
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG22	3	0.41
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG23	3	0.41
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG21	7	0.41
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG22	7	0.41
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG23	7	0.41
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG21	9	0.41
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG22	9	0.41
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG23	9	0.41
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG11	4	0.41
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG12	4	0.41
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG13	4	0.41
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG11	6	0.41
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG12	6	0.41
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG13	6	0.41
(1,14)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,69)	1:7:A:LEU:HB3	1:10:A:GLN:H	2	0.4
(3,69)	1:7:A:LEU:HB3	1:10:A:GLN:H	4	0.4
(3,59)	1:4:A:ALA:HB1	1:7:A:LEU:H	1	0.4
(3,59)	1:4:A:ALA:HB2	1:7:A:LEU:H	1	0.4
(3,59)	1:4:A:ALA:HB3	1:7:A:LEU:H	1	0.4
(3,48)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	6	0.4
(3,48)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	6	0.4
(3,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	5	0.4
(3,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	5	0.4
(3,35)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	1	0.4
(3,35)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	2	0.4
(3,35)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	3	0.4
(3,35)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	4	0.4
(3,35)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	8	0.4
(3,31)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	2	0.4
(3,31)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	2	0.4
(3,31)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	8	0.4
(3,31)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	8	0.4
(3,31)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	9	0.4
(3,31)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	9	0.4
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	4	0.4
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	4	0.4
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	4	0.4
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	8	0.4
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	8	0.4
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	8	0.4
(3,4)	1:3:A:GLU:H	1:3:A:GLU:HG3	8	0.4
(3,2)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	1	0.4
(3,2)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	5	0.4
(3,2)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	6	0.4
(3,2)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	7	0.4
(3,2)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	8	0.4
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	3	0.4
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	3	0.4
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	3	0.4
(2,529)	1:5:A:VAL:H	1:6:A:ARG:HB3	2	0.4
(2,221)	1:21:A:ARG:HA	1:21:A:ARG:HG2	7	0.4
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	3	0.4
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	3	0.4
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	3	0.4
(1,601)	1:5:A:VAL:H	1:6:A:ARG:HB3	2	0.4
(1,571)	1:7:A:LEU:HB3	1:10:A:GLN:H	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,571)	1:7:A:LEU:HB3	1:10:A:GLN:H	4	0.4
(1,498)	1:4:A:ALA:HB1	1:7:A:LEU:H	1	0.4
(1,498)	1:4:A:ALA:HB2	1:7:A:LEU:H	1	0.4
(1,498)	1:4:A:ALA:HB3	1:7:A:LEU:H	1	0.4
(1,457)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	6	0.4
(1,457)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	6	0.4
(1,350)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	5	0.4
(1,350)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	5	0.4
(1,342)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	1	0.4
(1,342)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	2	0.4
(1,342)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	3	0.4
(1,342)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	4	0.4
(1,342)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	8	0.4
(1,330)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	2	0.4
(1,330)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	2	0.4
(1,330)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	8	0.4
(1,330)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	8	0.4
(1,330)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	9	0.4
(1,330)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	9	0.4
(1,247)	1:21:A:ARG:HA	1:21:A:ARG:HG2	7	0.4
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG21	4	0.4
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG22	4	0.4
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG23	4	0.4
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG21	8	0.4
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG22	8	0.4
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG23	8	0.4
(1,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	8	0.4
(1,14)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	1	0.4
(1,14)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	5	0.4
(1,14)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	6	0.4
(1,14)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	7	0.4
(1,14)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	8	0.4
(3,59)	1:4:A:ALA:HB1	1:7:A:LEU:H	2	0.39
(3,59)	1:4:A:ALA:HB2	1:7:A:LEU:H	2	0.39
(3,59)	1:4:A:ALA:HB3	1:7:A:LEU:H	2	0.39
(3,59)	1:4:A:ALA:HB1	1:7:A:LEU:H	5	0.39
(3,59)	1:4:A:ALA:HB2	1:7:A:LEU:H	5	0.39
(3,59)	1:4:A:ALA:HB3	1:7:A:LEU:H	5	0.39
(3,59)	1:4:A:ALA:HB1	1:7:A:LEU:H	8	0.39
(3,59)	1:4:A:ALA:HB2	1:7:A:LEU:H	8	0.39
(3,59)	1:4:A:ALA:HB3	1:7:A:LEU:H	8	0.39
(3,59)	1:4:A:ALA:HB1	1:7:A:LEU:H	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,59)	1:4:A:ALA:HB2	1:7:A:LEU:H	10	0.39
(3,59)	1:4:A:ALA:HB3	1:7:A:LEU:H	10	0.39
(3,48)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	9	0.39
(3,48)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	9	0.39
(3,43)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	0.39
(3,43)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	0.39
(3,43)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	0.39
(3,43)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	0.39
(3,43)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.39
(3,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	7	0.39
(3,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	7	0.39
(3,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	8	0.39
(3,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	8	0.39
(3,33)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	0.39
(3,33)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG11	3	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG12	3	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG13	3	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG11	7	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG12	7	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG13	7	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG11	8	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG12	8	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG13	8	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG11	9	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG12	9	0.39
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG13	9	0.39
(3,2)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	2	0.39
(3,2)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	3	0.39
(3,2)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	10	0.39
(2,463)	1:17:A:PRO:HB3	1:19:A:SER:H	5	0.39
(2,463)	1:17:A:PRO:HB3	1:19:A:SER:H	7	0.39
(2,221)	1:21:A:ARG:HA	1:21:A:ARG:HG2	1	0.39
(2,208)	1:21:A:ARG:H	1:21:A:ARG:HD2	2	0.39
(2,160)	1:13:A:LYS:H	1:13:A:LYS:HG2	10	0.39
(1,526)	1:17:A:PRO:HB3	1:19:A:SER:H	5	0.39
(1,526)	1:17:A:PRO:HB3	1:19:A:SER:H	7	0.39
(1,498)	1:4:A:ALA:HB1	1:7:A:LEU:H	2	0.39
(1,498)	1:4:A:ALA:HB2	1:7:A:LEU:H	2	0.39
(1,498)	1:4:A:ALA:HB3	1:7:A:LEU:H	2	0.39
(1,498)	1:4:A:ALA:HB1	1:7:A:LEU:H	5	0.39
(1,498)	1:4:A:ALA:HB2	1:7:A:LEU:H	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:4:A:ALA:HB3	1:7:A:LEU:H	5	0.39
(1,498)	1:4:A:ALA:HB1	1:7:A:LEU:H	8	0.39
(1,498)	1:4:A:ALA:HB2	1:7:A:LEU:H	8	0.39
(1,498)	1:4:A:ALA:HB3	1:7:A:LEU:H	8	0.39
(1,498)	1:4:A:ALA:HB1	1:7:A:LEU:H	10	0.39
(1,498)	1:4:A:ALA:HB2	1:7:A:LEU:H	10	0.39
(1,498)	1:4:A:ALA:HB3	1:7:A:LEU:H	10	0.39
(1,457)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	9	0.39
(1,457)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	9	0.39
(1,396)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	0.39
(1,396)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	0.39
(1,396)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	0.39
(1,396)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	0.39
(1,396)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.39
(1,350)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	7	0.39
(1,350)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	7	0.39
(1,350)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	8	0.39
(1,350)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	8	0.39
(1,337)	1:8:A:TYR:HD1	1:12:A:LEU:HG	10	0.39
(1,337)	1:8:A:TYR:HD2	1:12:A:LEU:HG	10	0.39
(1,247)	1:21:A:ARG:HA	1:21:A:ARG:HG2	1	0.39
(1,233)	1:21:A:ARG:H	1:21:A:ARG:HD2	2	0.39
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	10	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG11	3	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG12	3	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG13	3	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG11	7	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG12	7	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG13	7	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG11	8	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG12	8	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG13	8	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG11	9	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG12	9	0.39
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG13	9	0.39
(1,14)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	2	0.39
(1,14)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	3	0.39
(1,14)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	10	0.39
(3,80)	1:17:A:PRO:HA	1:19:A:SER:H	5	0.38
(3,80)	1:17:A:PRO:HA	1:19:A:SER:H	6	0.38
(3,74)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	2	0.38
(3,59)	1:4:A:ALA:HB1	1:7:A:LEU:H	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,59)	1:4:A:ALA:HB2	1:7:A:LEU:H	4	0.38
(3,59)	1:4:A:ALA:HB3	1:7:A:LEU:H	4	0.38
(3,43)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	0.38
(3,43)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	0.38
(3,33)	1:8:A:TYR:HD1	1:12:A:LEU:HG	4	0.38
(3,33)	1:8:A:TYR:HD2	1:12:A:LEU:HG	4	0.38
(3,26)	1:21:A:ARG:H	1:21:A:ARG:HG2	10	0.38
(2,221)	1:21:A:ARG:HA	1:21:A:ARG:HG2	10	0.38
(1,747)	1:17:A:PRO:HA	1:19:A:SER:H	5	0.38
(1,747)	1:17:A:PRO:HA	1:19:A:SER:H	6	0.38
(1,667)	1:21:A:ARG:HB3	1:22:A:PRO:HD3	2	0.38
(1,498)	1:4:A:ALA:HB1	1:7:A:LEU:H	4	0.38
(1,498)	1:4:A:ALA:HB2	1:7:A:LEU:H	4	0.38
(1,498)	1:4:A:ALA:HB3	1:7:A:LEU:H	4	0.38
(1,396)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	0.38
(1,396)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	0.38
(1,337)	1:8:A:TYR:HD1	1:12:A:LEU:HG	4	0.38
(1,337)	1:8:A:TYR:HD2	1:12:A:LEU:HG	4	0.38
(1,247)	1:21:A:ARG:HA	1:21:A:ARG:HG2	10	0.38
(1,239)	1:21:A:ARG:H	1:21:A:ARG:HG2	10	0.38
(3,80)	1:17:A:PRO:HA	1:19:A:SER:H	2	0.37
(3,80)	1:17:A:PRO:HA	1:19:A:SER:H	8	0.37
(3,80)	1:17:A:PRO:HA	1:19:A:SER:H	9	0.37
(3,76)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	10	0.37
(3,76)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	10	0.37
(3,76)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	10	0.37
(3,48)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	4	0.37
(3,48)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	4	0.37
(3,48)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	10	0.37
(3,48)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	10	0.37
(3,46)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.37
(3,46)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.37
(3,43)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	0.37
(3,43)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	0.37
(3,36)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	6	0.37
(3,36)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	6	0.37
(3,26)	1:21:A:ARG:H	1:21:A:ARG:HG2	7	0.37
(3,19)	1:10:A:GLN:H	1:10:A:GLN:HG2	4	0.37
(3,19)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.37
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	1	0.37
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	1	0.37
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG11	1	0.37
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG12	1	0.37
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG13	1	0.37
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG11	2	0.37
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG12	2	0.37
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG13	2	0.37
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG11	5	0.37
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG12	5	0.37
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG13	5	0.37
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	1	0.37
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	1	0.37
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	8	0.37
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	8	0.37
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	9	0.37
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	9	0.37
(2,463)	1:17:A:PRO:HB3	1:19:A:SER:H	9	0.37
(2,160)	1:13:A:LYS:H	1:13:A:LYS:HG2	3	0.37
(1,747)	1:17:A:PRO:HA	1:19:A:SER:H	2	0.37
(1,747)	1:17:A:PRO:HA	1:19:A:SER:H	8	0.37
(1,747)	1:17:A:PRO:HA	1:19:A:SER:H	9	0.37
(1,717)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	10	0.37
(1,717)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	10	0.37
(1,717)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	10	0.37
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	1	0.37
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	1	0.37
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	8	0.37
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	8	0.37
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	9	0.37
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	9	0.37
(1,526)	1:17:A:PRO:HB3	1:19:A:SER:H	9	0.37
(1,457)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	4	0.37
(1,457)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	4	0.37
(1,457)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	10	0.37
(1,457)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	10	0.37
(1,443)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.37
(1,443)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.37
(1,396)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	0.37
(1,396)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	0.37
(1,350)	1:8:A:TYR:HE1	1:12:A:LEU:HB2	6	0.37
(1,350)	1:8:A:TYR:HE2	1:12:A:LEU:HB2	6	0.37
(1,239)	1:21:A:ARG:H	1:21:A:ARG:HG2	7	0.37
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:10:A:GLN:H	1:10:A:GLN:HG2	4	0.37
(1,127)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.37
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG21	1	0.37
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG22	1	0.37
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG23	1	0.37
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG11	1	0.37
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG12	1	0.37
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG13	1	0.37
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG11	2	0.37
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG12	2	0.37
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG13	2	0.37
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG11	5	0.37
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG12	5	0.37
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG13	5	0.37
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD11	7	0.36
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD12	7	0.36
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD13	7	0.36
(3,80)	1:17:A:PRO:HA	1:19:A:SER:H	3	0.36
(3,80)	1:17:A:PRO:HA	1:19:A:SER:H	4	0.36
(3,76)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	3	0.36
(3,76)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	3	0.36
(3,76)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	3	0.36
(3,76)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	9	0.36
(3,76)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	9	0.36
(3,76)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	9	0.36
(3,59)	1:4:A:ALA:HB1	1:7:A:LEU:H	6	0.36
(3,59)	1:4:A:ALA:HB2	1:7:A:LEU:H	6	0.36
(3,59)	1:4:A:ALA:HB3	1:7:A:LEU:H	6	0.36
(3,48)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	1	0.36
(3,48)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	1	0.36
(3,46)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.36
(3,46)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.36
(3,46)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.36
(3,46)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.36
(3,46)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.36
(3,46)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.36
(3,46)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.36
(3,30)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	5	0.36
(3,30)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	5	0.36
(3,26)	1:21:A:ARG:H	1:21:A:ARG:HG2	9	0.36
(3,19)	1:10:A:GLN:H	1:10:A:GLN:HG2	5	0.36
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	2	0.36
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	2	0.36
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	5	0.36
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	5	0.36
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	5	0.36
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.36
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.36
(3,7)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.36
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG11	10	0.36
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG12	10	0.36
(3,5)	1:5:A:VAL:HA	1:5:A:VAL:HG13	10	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	2	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	2	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	3	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	3	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	4	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	4	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	6	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	6	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	7	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	7	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	10	0.36
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	10	0.36
(2,510)	1:17:A:PRO:HB3	1:18:A:SER:H	7	0.36
(2,463)	1:17:A:PRO:HB3	1:19:A:SER:H	6	0.36
(2,463)	1:17:A:PRO:HB3	1:19:A:SER:H	8	0.36
(2,463)	1:17:A:PRO:HB3	1:19:A:SER:H	10	0.36
(2,250)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	2	0.36
(2,221)	1:21:A:ARG:HA	1:21:A:ARG:HG2	5	0.36
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD11	7	0.36
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD12	7	0.36
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD13	7	0.36
(1,747)	1:17:A:PRO:HA	1:19:A:SER:H	3	0.36
(1,747)	1:17:A:PRO:HA	1:19:A:SER:H	4	0.36
(1,717)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	3	0.36
(1,717)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	3	0.36
(1,717)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	3	0.36
(1,717)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	9	0.36
(1,717)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	9	0.36
(1,717)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	9	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	2	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	3	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	3	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	4	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	4	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	6	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	6	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	7	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	7	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	10	0.36
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	10	0.36
(1,581)	1:17:A:PRO:HB3	1:18:A:SER:H	7	0.36
(1,526)	1:17:A:PRO:HB3	1:19:A:SER:H	6	0.36
(1,526)	1:17:A:PRO:HB3	1:19:A:SER:H	8	0.36
(1,526)	1:17:A:PRO:HB3	1:19:A:SER:H	10	0.36
(1,498)	1:4:A:ALA:HB1	1:7:A:LEU:H	6	0.36
(1,498)	1:4:A:ALA:HB2	1:7:A:LEU:H	6	0.36
(1,498)	1:4:A:ALA:HB3	1:7:A:LEU:H	6	0.36
(1,457)	1:8:A:TYR:HE1	1:11:A:TRP:HZ2	1	0.36
(1,457)	1:8:A:TYR:HE2	1:11:A:TRP:HZ2	1	0.36
(1,443)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.36
(1,443)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.36
(1,443)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.36
(1,443)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.36
(1,443)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.36
(1,443)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.36
(1,443)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.36
(1,320)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	5	0.36
(1,320)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	5	0.36
(1,278)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	2	0.36
(1,247)	1:21:A:ARG:HA	1:21:A:ARG:HG2	5	0.36
(1,239)	1:21:A:ARG:H	1:21:A:ARG:HG2	9	0.36
(1,127)	1:10:A:GLN:H	1:10:A:GLN:HG2	5	0.36
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG21	2	0.36
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG22	2	0.36
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG23	2	0.36
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG21	5	0.36
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG22	5	0.36
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG23	5	0.36
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.36
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.36
(1,32)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.36
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG11	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG12	10	0.36
(1,26)	1:5:A:VAL:HA	1:5:A:VAL:HG13	10	0.36
(3,80)	1:17:A:PRO:HA	1:19:A:SER:H	1	0.35
(3,76)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	4	0.35
(3,76)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	4	0.35
(3,76)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	4	0.35
(3,76)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	7	0.35
(3,76)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	7	0.35
(3,76)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	7	0.35
(3,59)	1:4:A:ALA:HB1	1:7:A:LEU:H	3	0.35
(3,59)	1:4:A:ALA:HB2	1:7:A:LEU:H	3	0.35
(3,59)	1:4:A:ALA:HB3	1:7:A:LEU:H	3	0.35
(3,59)	1:4:A:ALA:HB1	1:7:A:LEU:H	9	0.35
(3,59)	1:4:A:ALA:HB2	1:7:A:LEU:H	9	0.35
(3,59)	1:4:A:ALA:HB3	1:7:A:LEU:H	9	0.35
(3,46)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.35
(3,33)	1:8:A:TYR:HD1	1:12:A:LEU:HG	1	0.35
(3,33)	1:8:A:TYR:HD2	1:12:A:LEU:HG	1	0.35
(3,26)	1:21:A:ARG:H	1:21:A:ARG:HG2	3	0.35
(3,26)	1:21:A:ARG:H	1:21:A:ARG:HG2	4	0.35
(3,26)	1:21:A:ARG:H	1:21:A:ARG:HG2	6	0.35
(3,26)	1:21:A:ARG:H	1:21:A:ARG:HG2	8	0.35
(3,19)	1:10:A:GLN:H	1:10:A:GLN:HG2	1	0.35
(3,19)	1:10:A:GLN:H	1:10:A:GLN:HG2	2	0.35
(3,19)	1:10:A:GLN:H	1:10:A:GLN:HG2	7	0.35
(3,19)	1:10:A:GLN:H	1:10:A:GLN:HG2	9	0.35
(2,529)	1:5:A:VAL:H	1:6:A:ARG:HB3	10	0.35
(2,160)	1:13:A:LYS:H	1:13:A:LYS:HG2	9	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	2	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	2	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	2	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	5	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	5	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	5	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	7	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	7	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	7	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	9	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	9	0.35
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	9	0.35
(1,747)	1:17:A:PRO:HA	1:19:A:SER:H	1	0.35
(1,717)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,717)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	4	0.35
(1,717)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	4	0.35
(1,717)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	7	0.35
(1,717)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	7	0.35
(1,717)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	7	0.35
(1,601)	1:5:A:VAL:H	1:6:A:ARG:HB3	10	0.35
(1,498)	1:4:A:ALA:HB1	1:7:A:LEU:H	3	0.35
(1,498)	1:4:A:ALA:HB2	1:7:A:LEU:H	3	0.35
(1,498)	1:4:A:ALA:HB3	1:7:A:LEU:H	3	0.35
(1,498)	1:4:A:ALA:HB1	1:7:A:LEU:H	9	0.35
(1,498)	1:4:A:ALA:HB2	1:7:A:LEU:H	9	0.35
(1,498)	1:4:A:ALA:HB3	1:7:A:LEU:H	9	0.35
(1,443)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.35
(1,337)	1:8:A:TYR:HD1	1:12:A:LEU:HG	1	0.35
(1,337)	1:8:A:TYR:HD2	1:12:A:LEU:HG	1	0.35
(1,239)	1:21:A:ARG:H	1:21:A:ARG:HG2	3	0.35
(1,239)	1:21:A:ARG:H	1:21:A:ARG:HG2	4	0.35
(1,239)	1:21:A:ARG:H	1:21:A:ARG:HG2	6	0.35
(1,239)	1:21:A:ARG:H	1:21:A:ARG:HG2	8	0.35
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	9	0.35
(1,127)	1:10:A:GLN:H	1:10:A:GLN:HG2	1	0.35
(1,127)	1:10:A:GLN:H	1:10:A:GLN:HG2	2	0.35
(1,127)	1:10:A:GLN:H	1:10:A:GLN:HG2	7	0.35
(1,127)	1:10:A:GLN:H	1:10:A:GLN:HG2	9	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	2	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	2	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	2	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	5	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	5	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	5	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	7	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	7	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	7	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	9	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	9	0.35
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	9	0.35
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD11	9	0.34
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD12	9	0.34
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD13	9	0.34
(3,80)	1:17:A:PRO:HA	1:19:A:SER:H	7	0.34
(3,80)	1:17:A:PRO:HA	1:19:A:SER:H	10	0.34
(3,76)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,76)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	5	0.34
(3,76)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	5	0.34
(3,76)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	8	0.34
(3,76)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	8	0.34
(3,76)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	8	0.34
(3,59)	1:4:A:ALA:HB1	1:7:A:LEU:H	7	0.34
(3,59)	1:4:A:ALA:HB2	1:7:A:LEU:H	7	0.34
(3,59)	1:4:A:ALA:HB3	1:7:A:LEU:H	7	0.34
(3,31)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	1	0.34
(3,31)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	1	0.34
(3,31)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	4	0.34
(3,31)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	4	0.34
(3,30)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	7	0.34
(3,30)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	7	0.34
(3,19)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.34
(3,19)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.34
(3,11)	1:7:A:LEU:HB2	1:7:A:LEU:HG	1	0.34
(3,11)	1:7:A:LEU:HB2	1:7:A:LEU:HG	2	0.34
(3,11)	1:7:A:LEU:HB2	1:7:A:LEU:HG	3	0.34
(3,11)	1:7:A:LEU:HB2	1:7:A:LEU:HG	5	0.34
(3,11)	1:7:A:LEU:HB2	1:7:A:LEU:HG	6	0.34
(3,11)	1:7:A:LEU:HB2	1:7:A:LEU:HG	7	0.34
(3,11)	1:7:A:LEU:HB2	1:7:A:LEU:HG	8	0.34
(3,11)	1:7:A:LEU:HB2	1:7:A:LEU:HG	9	0.34
(3,11)	1:7:A:LEU:HB2	1:7:A:LEU:HG	10	0.34
(2,607)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	7	0.34
(2,607)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	10	0.34
(2,463)	1:17:A:PRO:HB3	1:19:A:SER:H	3	0.34
(2,463)	1:17:A:PRO:HB3	1:19:A:SER:H	4	0.34
(2,250)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	1	0.34
(2,250)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	5	0.34
(2,250)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	7	0.34
(2,250)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	10	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	1	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	1	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	1	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	3	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	3	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	3	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	6	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	6	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	8	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	8	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	8	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.34
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.34
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD11	9	0.34
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD12	9	0.34
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD13	9	0.34
(1,747)	1:17:A:PRO:HA	1:19:A:SER:H	7	0.34
(1,747)	1:17:A:PRO:HA	1:19:A:SER:H	10	0.34
(1,717)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	5	0.34
(1,717)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	5	0.34
(1,717)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	5	0.34
(1,717)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	8	0.34
(1,717)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	8	0.34
(1,717)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	8	0.34
(1,681)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	7	0.34
(1,681)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	10	0.34
(1,526)	1:17:A:PRO:HB3	1:19:A:SER:H	3	0.34
(1,526)	1:17:A:PRO:HB3	1:19:A:SER:H	4	0.34
(1,498)	1:4:A:ALA:HB1	1:7:A:LEU:H	7	0.34
(1,498)	1:4:A:ALA:HB2	1:7:A:LEU:H	7	0.34
(1,498)	1:4:A:ALA:HB3	1:7:A:LEU:H	7	0.34
(1,330)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	1	0.34
(1,330)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	1	0.34
(1,330)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	4	0.34
(1,330)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	4	0.34
(1,320)	1:1:A:GLU:HB2	1:1:A:GLU:HG3	7	0.34
(1,320)	1:1:A:GLU:HB3	1:1:A:GLU:HG3	7	0.34
(1,278)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	1	0.34
(1,278)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	5	0.34
(1,278)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	7	0.34
(1,278)	1:22:A:PRO:HB3	1:22:A:PRO:HG2	10	0.34
(1,127)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.34
(1,127)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	1	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	1	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	1	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	3	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	3	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	6	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	6	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	6	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	8	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	8	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	8	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.34
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.34
(1,71)	1:7:A:LEU:HB2	1:7:A:LEU:HG	1	0.34
(1,71)	1:7:A:LEU:HB2	1:7:A:LEU:HG	2	0.34
(1,71)	1:7:A:LEU:HB2	1:7:A:LEU:HG	3	0.34
(1,71)	1:7:A:LEU:HB2	1:7:A:LEU:HG	5	0.34
(1,71)	1:7:A:LEU:HB2	1:7:A:LEU:HG	6	0.34
(1,71)	1:7:A:LEU:HB2	1:7:A:LEU:HG	7	0.34
(1,71)	1:7:A:LEU:HB2	1:7:A:LEU:HG	8	0.34
(1,71)	1:7:A:LEU:HB2	1:7:A:LEU:HG	9	0.34
(1,71)	1:7:A:LEU:HB2	1:7:A:LEU:HG	10	0.34
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD11	3	0.33
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD12	3	0.33
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD13	3	0.33
(3,76)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	6	0.33
(3,76)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	6	0.33
(3,76)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	6	0.33
(3,72)	1:3:A:GLU:HG2	1:5:A:VAL:H	9	0.33
(3,54)	1:16:A:GLY:H	1:17:A:PRO:HD2	5	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	1	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	1	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	1	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	3	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	3	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	3	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	7	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	7	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	7	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	8	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	8	0.33
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	8	0.33
(3,31)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	10	0.33
(3,31)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	10	0.33
(3,28)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	2	0.33
(3,28)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,28)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.33
(3,19)	1:10:A:GLN:H	1:10:A:GLN:HG2	8	0.33
(3,11)	1:7:A:LEU:HB2	1:7:A:LEU:HG	4	0.33
(2,607)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	5	0.33
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	5	0.33
(2,605)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	5	0.33
(2,510)	1:17:A:PRO:HB3	1:18:A:SER:H	5	0.33
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	4	0.33
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	4	0.33
(2,89)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	4	0.33
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD11	3	0.33
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD12	3	0.33
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD13	3	0.33
(1,717)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	6	0.33
(1,717)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	6	0.33
(1,717)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	6	0.33
(1,681)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	5	0.33
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	5	0.33
(1,679)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	5	0.33
(1,599)	1:3:A:GLU:HG2	1:5:A:VAL:H	9	0.33
(1,581)	1:17:A:PRO:HB3	1:18:A:SER:H	5	0.33
(1,478)	1:16:A:GLY:H	1:17:A:PRO:HD2	5	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	1	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	1	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	1	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	3	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	3	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	3	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	7	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	7	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	7	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	8	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	8	0.33
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	8	0.33
(1,330)	1:8:A:TYR:HD1	1:11:A:TRP:HB2	10	0.33
(1,330)	1:8:A:TYR:HD2	1:11:A:TRP:HB2	10	0.33
(1,274)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	2	0.33
(1,274)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	7	0.33
(1,274)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.33
(1,127)	1:10:A:GLN:H	1:10:A:GLN:HG2	8	0.33
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	4	0.33
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	4	0.33
(1,71)	1:7:A:LEU:HB2	1:7:A:LEU:HG	4	0.33
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD11	4	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD12	4	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD13	4	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD11	5	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD12	5	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD13	5	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD11	6	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD12	6	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD13	6	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD11	8	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD12	8	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD13	8	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD11	10	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD12	10	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD13	10	0.32
(3,76)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	1	0.32
(3,76)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	1	0.32
(3,76)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	1	0.32
(3,54)	1:16:A:GLY:H	1:17:A:PRO:HD2	3	0.32
(3,54)	1:16:A:GLY:H	1:17:A:PRO:HD2	4	0.32
(3,54)	1:16:A:GLY:H	1:17:A:PRO:HD2	7	0.32
(3,54)	1:16:A:GLY:H	1:17:A:PRO:HD2	10	0.32
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	1	0.32
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	1	0.32
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	5	0.32
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	5	0.32
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.32
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.32
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.32
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	9	0.32
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	9	0.32
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	9	0.32
(3,28)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	1	0.32
(3,28)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	5	0.32
(2,463)	1:17:A:PRO:HB3	1:19:A:SER:H	1	0.32
(2,463)	1:17:A:PRO:HB3	1:19:A:SER:H	2	0.32
(2,160)	1:13:A:LYS:H	1:13:A:LYS:HG2	5	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD11	4	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD12	4	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD13	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD11	5	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD12	5	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD13	5	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD11	6	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD12	6	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD13	6	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD11	8	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD12	8	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD13	8	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD11	10	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD12	10	0.32
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD13	10	0.32
(1,717)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	1	0.32
(1,717)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	1	0.32
(1,717)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	1	0.32
(1,526)	1:17:A:PRO:HB3	1:19:A:SER:H	1	0.32
(1,526)	1:17:A:PRO:HB3	1:19:A:SER:H	2	0.32
(1,478)	1:16:A:GLY:H	1:17:A:PRO:HD2	3	0.32
(1,478)	1:16:A:GLY:H	1:17:A:PRO:HD2	4	0.32
(1,478)	1:16:A:GLY:H	1:17:A:PRO:HD2	7	0.32
(1,478)	1:16:A:GLY:H	1:17:A:PRO:HD2	10	0.32
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	1	0.32
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	1	0.32
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	5	0.32
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	5	0.32
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	2	0.32
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	2	0.32
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	2	0.32
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	9	0.32
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	9	0.32
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	9	0.32
(1,274)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	1	0.32
(1,274)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	5	0.32
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	5	0.32
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD11	1	0.31
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD12	1	0.31
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD13	1	0.31
(3,76)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	2	0.31
(3,76)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	2	0.31
(3,76)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	2	0.31
(3,55)	1:16:A:GLY:H	1:17:A:PRO:HD3	1	0.31
(3,55)	1:16:A:GLY:H	1:17:A:PRO:HD3	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,54)	1:16:A:GLY:H	1:17:A:PRO:HD2	1	0.31
(3,54)	1:16:A:GLY:H	1:17:A:PRO:HD2	2	0.31
(3,54)	1:16:A:GLY:H	1:17:A:PRO:HD2	8	0.31
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	6	0.31
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	6	0.31
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	8	0.31
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	8	0.31
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	4	0.31
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	4	0.31
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	4	0.31
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	6	0.31
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	6	0.31
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	6	0.31
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.31
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.31
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.31
(2,185)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	7	0.31
(2,160)	1:13:A:LYS:H	1:13:A:LYS:HG2	7	0.31
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD11	1	0.31
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD12	1	0.31
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD13	1	0.31
(1,717)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	2	0.31
(1,717)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	2	0.31
(1,717)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	2	0.31
(1,481)	1:16:A:GLY:H	1:17:A:PRO:HD3	1	0.31
(1,481)	1:16:A:GLY:H	1:17:A:PRO:HD3	3	0.31
(1,478)	1:16:A:GLY:H	1:17:A:PRO:HD2	1	0.31
(1,478)	1:16:A:GLY:H	1:17:A:PRO:HD2	2	0.31
(1,478)	1:16:A:GLY:H	1:17:A:PRO:HD2	8	0.31
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	6	0.31
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	6	0.31
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	8	0.31
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	8	0.31
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	4	0.31
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	4	0.31
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	4	0.31
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	6	0.31
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	6	0.31
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	6	0.31
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	10	0.31
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	10	0.31
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	7	0.31
(1,183)	1:13:A:LYS:H	1:13:A:LYS:HG2	7	0.31
(3,83)	1:5:A:VAL:HG21	1:9:A:ILE:HB	5	0.3
(3,83)	1:5:A:VAL:HG22	1:9:A:ILE:HB	5	0.3
(3,83)	1:5:A:VAL:HG23	1:9:A:ILE:HB	5	0.3
(3,83)	1:5:A:VAL:HG21	1:9:A:ILE:HB	7	0.3
(3,83)	1:5:A:VAL:HG22	1:9:A:ILE:HB	7	0.3
(3,83)	1:5:A:VAL:HG23	1:9:A:ILE:HB	7	0.3
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD11	2	0.3
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD12	2	0.3
(3,81)	1:4:A:ALA:HA	1:7:A:LEU:HD13	2	0.3
(3,55)	1:16:A:GLY:H	1:17:A:PRO:HD3	2	0.3
(3,55)	1:16:A:GLY:H	1:17:A:PRO:HD3	4	0.3
(3,55)	1:16:A:GLY:H	1:17:A:PRO:HD3	6	0.3
(3,55)	1:16:A:GLY:H	1:17:A:PRO:HD3	7	0.3
(3,55)	1:16:A:GLY:H	1:17:A:PRO:HD3	9	0.3
(3,55)	1:16:A:GLY:H	1:17:A:PRO:HD3	10	0.3
(3,54)	1:16:A:GLY:H	1:17:A:PRO:HD2	6	0.3
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	3	0.3
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	3	0.3
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	4	0.3
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	4	0.3
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	9	0.3
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	9	0.3
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	10	0.3
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	10	0.3
(2,607)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	1	0.3
(2,510)	1:17:A:PRO:HB3	1:18:A:SER:H	8	0.3
(2,362)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	2	0.3
(2,316)	1:8:A:TYR:HD1	1:9:A:ILE:HB	5	0.3
(2,316)	1:8:A:TYR:HD2	1:9:A:ILE:HB	5	0.3
(2,185)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	3	0.3
(2,185)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	5	0.3
(2,185)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	6	0.3
(2,185)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	9	0.3
(2,185)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	10	0.3
(1,786)	1:5:A:VAL:HG21	1:9:A:ILE:HB	5	0.3
(1,786)	1:5:A:VAL:HG22	1:9:A:ILE:HB	5	0.3
(1,786)	1:5:A:VAL:HG23	1:9:A:ILE:HB	5	0.3
(1,786)	1:5:A:VAL:HG21	1:9:A:ILE:HB	7	0.3
(1,786)	1:5:A:VAL:HG22	1:9:A:ILE:HB	7	0.3
(1,786)	1:5:A:VAL:HG23	1:9:A:ILE:HB	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD11	2	0.3
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD12	2	0.3
(1,765)	1:4:A:ALA:HA	1:7:A:LEU:HD13	2	0.3
(1,681)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	1	0.3
(1,581)	1:17:A:PRO:HB3	1:18:A:SER:H	8	0.3
(1,481)	1:16:A:GLY:H	1:17:A:PRO:HD3	2	0.3
(1,481)	1:16:A:GLY:H	1:17:A:PRO:HD3	4	0.3
(1,481)	1:16:A:GLY:H	1:17:A:PRO:HD3	6	0.3
(1,481)	1:16:A:GLY:H	1:17:A:PRO:HD3	7	0.3
(1,481)	1:16:A:GLY:H	1:17:A:PRO:HD3	9	0.3
(1,481)	1:16:A:GLY:H	1:17:A:PRO:HD3	10	0.3
(1,478)	1:16:A:GLY:H	1:17:A:PRO:HD2	6	0.3
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	3	0.3
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	3	0.3
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	4	0.3
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	4	0.3
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	9	0.3
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	9	0.3
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	10	0.3
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	10	0.3
(1,405)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	2	0.3
(1,352)	1:8:A:TYR:HD1	1:9:A:ILE:HB	5	0.3
(1,352)	1:8:A:TYR:HD2	1:9:A:ILE:HB	5	0.3
(1,209)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	3	0.3
(1,209)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	5	0.3
(1,209)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	6	0.3
(1,209)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	9	0.3
(1,209)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	10	0.3
(3,83)	1:5:A:VAL:HG21	1:9:A:ILE:HB	3	0.29
(3,83)	1:5:A:VAL:HG22	1:9:A:ILE:HB	3	0.29
(3,83)	1:5:A:VAL:HG23	1:9:A:ILE:HB	3	0.29
(3,83)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	0.29
(3,83)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	0.29
(3,83)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	0.29
(3,66)	1:14:A:ASP:H	1:15:A:GLY:HA3	4	0.29
(3,66)	1:14:A:ASP:H	1:15:A:GLY:HA3	5	0.29
(3,54)	1:16:A:GLY:H	1:17:A:PRO:HD2	9	0.29
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	5	0.29
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	5	0.29
(3,45)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	5	0.29
(2,510)	1:17:A:PRO:HB3	1:18:A:SER:H	10	0.29
(2,316)	1:8:A:TYR:HD1	1:9:A:ILE:HB	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,316)	1:8:A:TYR:HD2	1:9:A:ILE:HB	2	0.29
(2,316)	1:8:A:TYR:HD1	1:9:A:ILE:HB	6	0.29
(2,316)	1:8:A:TYR:HD2	1:9:A:ILE:HB	6	0.29
(2,316)	1:8:A:TYR:HD1	1:9:A:ILE:HB	8	0.29
(2,316)	1:8:A:TYR:HD2	1:9:A:ILE:HB	8	0.29
(2,316)	1:8:A:TYR:HD1	1:9:A:ILE:HB	9	0.29
(2,316)	1:8:A:TYR:HD2	1:9:A:ILE:HB	9	0.29
(2,185)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	1	0.29
(2,185)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	4	0.29
(2,185)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	8	0.29
(1,786)	1:5:A:VAL:HG21	1:9:A:ILE:HB	3	0.29
(1,786)	1:5:A:VAL:HG22	1:9:A:ILE:HB	3	0.29
(1,786)	1:5:A:VAL:HG23	1:9:A:ILE:HB	3	0.29
(1,786)	1:5:A:VAL:HG21	1:9:A:ILE:HB	10	0.29
(1,786)	1:5:A:VAL:HG22	1:9:A:ILE:HB	10	0.29
(1,786)	1:5:A:VAL:HG23	1:9:A:ILE:HB	10	0.29
(1,581)	1:17:A:PRO:HB3	1:18:A:SER:H	10	0.29
(1,552)	1:14:A:ASP:H	1:15:A:GLY:HA3	4	0.29
(1,552)	1:14:A:ASP:H	1:15:A:GLY:HA3	5	0.29
(1,478)	1:16:A:GLY:H	1:17:A:PRO:HD2	9	0.29
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD11	5	0.29
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD12	5	0.29
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HD13	5	0.29
(1,352)	1:8:A:TYR:HD1	1:9:A:ILE:HB	2	0.29
(1,352)	1:8:A:TYR:HD2	1:9:A:ILE:HB	2	0.29
(1,352)	1:8:A:TYR:HD1	1:9:A:ILE:HB	6	0.29
(1,352)	1:8:A:TYR:HD2	1:9:A:ILE:HB	6	0.29
(1,352)	1:8:A:TYR:HD1	1:9:A:ILE:HB	8	0.29
(1,352)	1:8:A:TYR:HD2	1:9:A:ILE:HB	8	0.29
(1,352)	1:8:A:TYR:HD1	1:9:A:ILE:HB	9	0.29
(1,352)	1:8:A:TYR:HD2	1:9:A:ILE:HB	9	0.29
(1,209)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	1	0.29
(1,209)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	4	0.29
(1,209)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	8	0.29
(3,83)	1:5:A:VAL:HG21	1:9:A:ILE:HB	4	0.28
(3,83)	1:5:A:VAL:HG22	1:9:A:ILE:HB	4	0.28
(3,83)	1:5:A:VAL:HG23	1:9:A:ILE:HB	4	0.28
(3,83)	1:5:A:VAL:HG21	1:9:A:ILE:HB	6	0.28
(3,83)	1:5:A:VAL:HG22	1:9:A:ILE:HB	6	0.28
(3,83)	1:5:A:VAL:HG23	1:9:A:ILE:HB	6	0.28
(3,66)	1:14:A:ASP:H	1:15:A:GLY:HA3	3	0.28
(3,66)	1:14:A:ASP:H	1:15:A:GLY:HA3	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,66)	1:14:A:ASP:H	1:15:A:GLY:HA3	7	0.28
(3,55)	1:16:A:GLY:H	1:17:A:PRO:HD3	8	0.28
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	4	0.28
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	4	0.28
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	4	0.28
(2,607)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	2	0.28
(2,510)	1:17:A:PRO:HB3	1:18:A:SER:H	9	0.28
(2,185)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	2	0.28
(1,786)	1:5:A:VAL:HG21	1:9:A:ILE:HB	4	0.28
(1,786)	1:5:A:VAL:HG22	1:9:A:ILE:HB	4	0.28
(1,786)	1:5:A:VAL:HG23	1:9:A:ILE:HB	4	0.28
(1,786)	1:5:A:VAL:HG21	1:9:A:ILE:HB	6	0.28
(1,786)	1:5:A:VAL:HG22	1:9:A:ILE:HB	6	0.28
(1,786)	1:5:A:VAL:HG23	1:9:A:ILE:HB	6	0.28
(1,728)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	4	0.28
(1,728)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	4	0.28
(1,728)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	4	0.28
(1,681)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	2	0.28
(1,581)	1:17:A:PRO:HB3	1:18:A:SER:H	9	0.28
(1,552)	1:14:A:ASP:H	1:15:A:GLY:HA3	3	0.28
(1,552)	1:14:A:ASP:H	1:15:A:GLY:HA3	6	0.28
(1,552)	1:14:A:ASP:H	1:15:A:GLY:HA3	7	0.28
(1,481)	1:16:A:GLY:H	1:17:A:PRO:HD3	8	0.28
(1,209)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	2	0.28
(3,83)	1:5:A:VAL:HG21	1:9:A:ILE:HB	1	0.27
(3,83)	1:5:A:VAL:HG22	1:9:A:ILE:HB	1	0.27
(3,83)	1:5:A:VAL:HG23	1:9:A:ILE:HB	1	0.27
(3,83)	1:5:A:VAL:HG21	1:9:A:ILE:HB	8	0.27
(3,83)	1:5:A:VAL:HG22	1:9:A:ILE:HB	8	0.27
(3,83)	1:5:A:VAL:HG23	1:9:A:ILE:HB	8	0.27
(3,83)	1:5:A:VAL:HG21	1:9:A:ILE:HB	9	0.27
(3,83)	1:5:A:VAL:HG22	1:9:A:ILE:HB	9	0.27
(3,83)	1:5:A:VAL:HG23	1:9:A:ILE:HB	9	0.27
(3,66)	1:14:A:ASP:H	1:15:A:GLY:HA3	1	0.27
(3,66)	1:14:A:ASP:H	1:15:A:GLY:HA3	2	0.27
(3,66)	1:14:A:ASP:H	1:15:A:GLY:HA3	8	0.27
(3,66)	1:14:A:ASP:H	1:15:A:GLY:HA3	10	0.27
(3,55)	1:16:A:GLY:H	1:17:A:PRO:HD3	5	0.27
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	2	0.27
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	2	0.27
(3,25)	1:19:A:SER:H	1:19:A:SER:HB2	2	0.27
(3,25)	1:19:A:SER:H	1:19:A:SER:HB2	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,25)	1:19:A:SER:H	1:19:A:SER:HB2	7	0.27
(3,25)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.27
(3,22)	1:10:A:GLN:HA	1:13:A:LYS:H	8	0.27
(2,362)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	1	0.27
(2,362)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	4	0.27
(2,362)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	6	0.27
(2,316)	1:8:A:TYR:HD1	1:9:A:ILE:HB	3	0.27
(2,316)	1:8:A:TYR:HD2	1:9:A:ILE:HB	3	0.27
(2,316)	1:8:A:TYR:HD1	1:9:A:ILE:HB	7	0.27
(2,316)	1:8:A:TYR:HD2	1:9:A:ILE:HB	7	0.27
(1,786)	1:5:A:VAL:HG21	1:9:A:ILE:HB	1	0.27
(1,786)	1:5:A:VAL:HG22	1:9:A:ILE:HB	1	0.27
(1,786)	1:5:A:VAL:HG23	1:9:A:ILE:HB	1	0.27
(1,786)	1:5:A:VAL:HG21	1:9:A:ILE:HB	8	0.27
(1,786)	1:5:A:VAL:HG22	1:9:A:ILE:HB	8	0.27
(1,786)	1:5:A:VAL:HG23	1:9:A:ILE:HB	8	0.27
(1,786)	1:5:A:VAL:HG21	1:9:A:ILE:HB	9	0.27
(1,786)	1:5:A:VAL:HG22	1:9:A:ILE:HB	9	0.27
(1,786)	1:5:A:VAL:HG23	1:9:A:ILE:HB	9	0.27
(1,552)	1:14:A:ASP:H	1:15:A:GLY:HA3	1	0.27
(1,552)	1:14:A:ASP:H	1:15:A:GLY:HA3	2	0.27
(1,552)	1:14:A:ASP:H	1:15:A:GLY:HA3	8	0.27
(1,552)	1:14:A:ASP:H	1:15:A:GLY:HA3	10	0.27
(1,481)	1:16:A:GLY:H	1:17:A:PRO:HD3	5	0.27
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	2	0.27
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	2	0.27
(1,405)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	1	0.27
(1,405)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	4	0.27
(1,405)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	6	0.27
(1,352)	1:8:A:TYR:HD1	1:9:A:ILE:HB	3	0.27
(1,352)	1:8:A:TYR:HD2	1:9:A:ILE:HB	3	0.27
(1,352)	1:8:A:TYR:HD1	1:9:A:ILE:HB	7	0.27
(1,352)	1:8:A:TYR:HD2	1:9:A:ILE:HB	7	0.27
(1,216)	1:19:A:SER:H	1:19:A:SER:HB2	2	0.27
(1,216)	1:19:A:SER:H	1:19:A:SER:HB2	5	0.27
(1,216)	1:19:A:SER:H	1:19:A:SER:HB2	7	0.27
(1,216)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.27
(1,165)	1:10:A:GLN:HA	1:13:A:LYS:H	8	0.27
(3,66)	1:14:A:ASP:H	1:15:A:GLY:HA3	9	0.26
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	7	0.26
(3,47)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	7	0.26
(3,25)	1:19:A:SER:H	1:19:A:SER:HB2	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,25)	1:19:A:SER:H	1:19:A:SER:HB2	3	0.26
(3,25)	1:19:A:SER:H	1:19:A:SER:HB2	4	0.26
(3,25)	1:19:A:SER:H	1:19:A:SER:HB2	6	0.26
(3,25)	1:19:A:SER:H	1:19:A:SER:HB2	8	0.26
(3,25)	1:19:A:SER:H	1:19:A:SER:HB2	9	0.26
(3,22)	1:10:A:GLN:HA	1:13:A:LYS:H	3	0.26
(3,22)	1:10:A:GLN:HA	1:13:A:LYS:H	7	0.26
(3,22)	1:10:A:GLN:HA	1:13:A:LYS:H	9	0.26
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	9	0.26
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	9	0.26
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	9	0.26
(2,510)	1:17:A:PRO:HB3	1:18:A:SER:H	6	0.26
(2,362)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	8	0.26
(2,362)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	9	0.26
(2,359)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	1	0.26
(2,287)	1:1:A:GLU:HA	1:1:A:GLU:HG2	9	0.26
(1,728)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	9	0.26
(1,728)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	9	0.26
(1,728)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	9	0.26
(1,581)	1:17:A:PRO:HB3	1:18:A:SER:H	6	0.26
(1,552)	1:14:A:ASP:H	1:15:A:GLY:HA3	9	0.26
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH11	7	0.26
(1,444)	1:11:A:TRP:HE1	1:21:A:ARG:HH12	7	0.26
(1,405)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	8	0.26
(1,405)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	9	0.26
(1,402)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	1	0.26
(1,316)	1:1:A:GLU:HA	1:1:A:GLU:HG2	9	0.26
(1,216)	1:19:A:SER:H	1:19:A:SER:HB2	1	0.26
(1,216)	1:19:A:SER:H	1:19:A:SER:HB2	3	0.26
(1,216)	1:19:A:SER:H	1:19:A:SER:HB2	4	0.26
(1,216)	1:19:A:SER:H	1:19:A:SER:HB2	6	0.26
(1,216)	1:19:A:SER:H	1:19:A:SER:HB2	8	0.26
(1,216)	1:19:A:SER:H	1:19:A:SER:HB2	9	0.26
(1,165)	1:10:A:GLN:HA	1:13:A:LYS:H	3	0.26
(1,165)	1:10:A:GLN:HA	1:13:A:LYS:H	7	0.26
(1,165)	1:10:A:GLN:HA	1:13:A:LYS:H	9	0.26
(3,83)	1:5:A:VAL:HG21	1:9:A:ILE:HB	2	0.25
(3,83)	1:5:A:VAL:HG22	1:9:A:ILE:HB	2	0.25
(3,83)	1:5:A:VAL:HG23	1:9:A:ILE:HB	2	0.25
(3,56)	1:7:A:LEU:H	1:10:A:GLN:HB2	8	0.25
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.25
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,22)	1:10:A:GLN:HA	1:13:A:LYS:H	6	0.25
(3,22)	1:10:A:GLN:HA	1:13:A:LYS:H	10	0.25
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	0.25
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	0.25
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	0.25
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	3	0.25
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	3	0.25
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	3	0.25
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	6	0.25
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	6	0.25
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	6	0.25
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	8	0.25
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	8	0.25
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	8	0.25
(2,510)	1:17:A:PRO:HB3	1:18:A:SER:H	4	0.25
(2,391)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	2	0.25
(2,391)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	6	0.25
(2,362)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	3	0.25
(2,359)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	2	0.25
(1,786)	1:5:A:VAL:HG21	1:9:A:ILE:HB	2	0.25
(1,786)	1:5:A:VAL:HG22	1:9:A:ILE:HB	2	0.25
(1,786)	1:5:A:VAL:HG23	1:9:A:ILE:HB	2	0.25
(1,728)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	1	0.25
(1,728)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	1	0.25
(1,728)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	1	0.25
(1,728)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	3	0.25
(1,728)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	3	0.25
(1,728)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	3	0.25
(1,728)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	6	0.25
(1,728)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	6	0.25
(1,728)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	6	0.25
(1,728)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	8	0.25
(1,728)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	8	0.25
(1,728)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	8	0.25
(1,581)	1:17:A:PRO:HB3	1:18:A:SER:H	4	0.25
(1,493)	1:7:A:LEU:H	1:10:A:GLN:HB2	8	0.25
(1,435)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	2	0.25
(1,435)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	6	0.25
(1,405)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	3	0.25
(1,402)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	2	0.25
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.25
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:10:A:GLN:HA	1:13:A:LYS:H	6	0.25
(1,165)	1:10:A:GLN:HA	1:13:A:LYS:H	10	0.25
(3,56)	1:7:A:LEU:H	1:10:A:GLN:HB2	6	0.24
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.24
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.24
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.24
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.24
(3,22)	1:10:A:GLN:HA	1:13:A:LYS:H	1	0.24
(3,22)	1:10:A:GLN:HA	1:13:A:LYS:H	4	0.24
(3,22)	1:10:A:GLN:HA	1:13:A:LYS:H	5	0.24
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.24
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.24
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.24
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.24
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.24
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.24
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	7	0.24
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	7	0.24
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	7	0.24
(2,391)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	9	0.24
(2,391)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.24
(2,362)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	10	0.24
(2,359)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	3	0.24
(2,359)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	5	0.24
(2,359)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	8	0.24
(2,359)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	9	0.24
(1,728)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	7	0.24
(1,728)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	7	0.24
(1,728)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	7	0.24
(1,493)	1:7:A:LEU:H	1:10:A:GLN:HB2	6	0.24
(1,435)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	9	0.24
(1,435)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.24
(1,405)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	10	0.24
(1,402)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	3	0.24
(1,402)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	5	0.24
(1,402)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	8	0.24
(1,402)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	9	0.24
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.24
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.24
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.24
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.24
(1,165)	1:10:A:GLN:HA	1:13:A:LYS:H	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:10:A:GLN:HA	1:13:A:LYS:H	4	0.24
(1,165)	1:10:A:GLN:HA	1:13:A:LYS:H	5	0.24
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.24
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.24
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.24
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.24
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.24
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.24
(3,26)	1:21:A:ARG:H	1:21:A:ARG:HG2	2	0.23
(3,22)	1:10:A:GLN:HA	1:13:A:LYS:H	2	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.23
(3,17)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.23
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	2	0.23
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	2	0.23
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	2	0.23
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.23
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.23
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.23
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	9	0.23
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,644)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	9	0.23
(2,391)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	7	0.23
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	2	0.23
(2,373)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	2	0.23
(2,287)	1:1:A:GLU:HA	1:1:A:GLU:HG2	8	0.23
(1,728)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	2	0.23
(1,728)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	2	0.23
(1,728)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	2	0.23
(1,728)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	10	0.23
(1,728)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	10	0.23
(1,728)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	10	0.23
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG21	9	0.23
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG22	9	0.23
(1,720)	1:1:A:GLU:HG2	1:5:A:VAL:HG23	9	0.23
(1,435)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	7	0.23
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH11	2	0.23
(1,416)	1:21:A:ARG:HG3	1:21:A:ARG:HH12	2	0.23
(1,316)	1:1:A:GLU:HA	1:1:A:GLU:HG2	8	0.23
(1,239)	1:21:A:ARG:H	1:21:A:ARG:HG2	2	0.23
(1,165)	1:10:A:GLN:HA	1:13:A:LYS:H	2	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.23
(1,109)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.23
(3,79)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	1	0.22
(3,79)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	1	0.22
(3,79)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	4	0.22
(3,79)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	4	0.22
(3,65)	1:5:A:VAL:HA	1:6:A:ARG:H	4	0.22
(3,56)	1:7:A:LEU:H	1:10:A:GLN:HB2	1	0.22
(3,56)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.22
(3,56)	1:7:A:LEU:H	1:10:A:GLN:HB2	3	0.22
(3,56)	1:7:A:LEU:H	1:10:A:GLN:HB2	4	0.22
(3,21)	1:12:A:LEU:H	1:12:A:LEU:HB3	1	0.22
(3,21)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.22
(2,607)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	4	0.22
(2,607)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	8	0.22
(2,599)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	1	0.22
(2,599)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	2	0.22
(2,599)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	8	0.22
(2,599)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	9	0.22
(2,514)	1:24:A:PRO:HD3	1:25:A:SER:H	7	0.22
(2,510)	1:17:A:PRO:HB3	1:18:A:SER:H	3	0.22
(2,507)	1:23:A:PRO:HB3	1:25:A:SER:H	9	0.22
(2,391)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	8	0.22
(2,287)	1:1:A:GLU:HA	1:1:A:GLU:HG2	1	0.22
(2,202)	1:18:A:SER:H	1:18:A:SER:HB3	1	0.22
(2,202)	1:18:A:SER:H	1:18:A:SER:HB3	6	0.22
(2,202)	1:18:A:SER:H	1:18:A:SER:HB3	9	0.22
(1,742)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	1	0.22
(1,742)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	1	0.22
(1,742)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	4	0.22
(1,742)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	4	0.22
(1,681)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	4	0.22
(1,681)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	8	0.22
(1,673)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	1	0.22
(1,673)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	2	0.22
(1,673)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	8	0.22
(1,673)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	9	0.22
(1,585)	1:24:A:PRO:HD3	1:25:A:SER:H	7	0.22
(1,581)	1:17:A:PRO:HB3	1:18:A:SER:H	3	0.22
(1,577)	1:23:A:PRO:HB3	1:25:A:SER:H	9	0.22
(1,548)	1:5:A:VAL:HA	1:6:A:ARG:H	4	0.22
(1,493)	1:7:A:LEU:H	1:10:A:GLN:HB2	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.22
(1,493)	1:7:A:LEU:H	1:10:A:GLN:HB2	3	0.22
(1,493)	1:7:A:LEU:H	1:10:A:GLN:HB2	4	0.22
(1,435)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	8	0.22
(1,316)	1:1:A:GLU:HA	1:1:A:GLU:HG2	1	0.22
(1,227)	1:18:A:SER:H	1:18:A:SER:HB3	1	0.22
(1,227)	1:18:A:SER:H	1:18:A:SER:HB3	6	0.22
(1,227)	1:18:A:SER:H	1:18:A:SER:HB3	9	0.22
(1,161)	1:12:A:LEU:H	1:12:A:LEU:HB3	1	0.22
(1,161)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.22
(3,79)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	10	0.21
(3,79)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	10	0.21
(3,67)	1:10:A:GLN:HB2	1:11:A:TRP:H	8	0.21
(3,65)	1:5:A:VAL:HA	1:6:A:ARG:H	1	0.21
(3,65)	1:5:A:VAL:HA	1:6:A:ARG:H	2	0.21
(3,65)	1:5:A:VAL:HA	1:6:A:ARG:H	3	0.21
(3,65)	1:5:A:VAL:HA	1:6:A:ARG:H	5	0.21
(3,65)	1:5:A:VAL:HA	1:6:A:ARG:H	8	0.21
(3,56)	1:7:A:LEU:H	1:10:A:GLN:HB2	5	0.21
(3,56)	1:7:A:LEU:H	1:10:A:GLN:HB2	9	0.21
(3,56)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.21
(3,24)	1:13:A:LYS:HA	1:14:A:ASP:H	6	0.21
(3,21)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.21
(2,651)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	5	0.21
(2,651)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	5	0.21
(2,651)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	5	0.21
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	3	0.21
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	3	0.21
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	3	0.21
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	7	0.21
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	7	0.21
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	7	0.21
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	8	0.21
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	8	0.21
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	8	0.21
(2,607)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	3	0.21
(2,607)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	6	0.21
(2,599)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	3	0.21
(2,599)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	4	0.21
(2,510)	1:17:A:PRO:HB3	1:18:A:SER:H	1	0.21
(2,470)	1:18:A:SER:HB3	1:19:A:SER:H	2	0.21
(2,470)	1:18:A:SER:HB3	1:19:A:SER:H	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,470)	1:18:A:SER:HB3	1:19:A:SER:H	6	0.21
(2,470)	1:18:A:SER:HB3	1:19:A:SER:H	9	0.21
(2,359)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	4	0.21
(2,316)	1:8:A:TYR:HD1	1:9:A:ILE:HB	1	0.21
(2,316)	1:8:A:TYR:HD2	1:9:A:ILE:HB	1	0.21
(2,287)	1:1:A:GLU:HA	1:1:A:GLU:HG2	3	0.21
(2,287)	1:1:A:GLU:HA	1:1:A:GLU:HG2	4	0.21
(2,202)	1:18:A:SER:H	1:18:A:SER:HB3	2	0.21
(2,202)	1:18:A:SER:H	1:18:A:SER:HB3	3	0.21
(2,202)	1:18:A:SER:H	1:18:A:SER:HB3	4	0.21
(2,202)	1:18:A:SER:H	1:18:A:SER:HB3	10	0.21
(1,742)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	10	0.21
(1,742)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	10	0.21
(1,728)	1:5:A:VAL:HG21	1:9:A:ILE:HG12	5	0.21
(1,728)	1:5:A:VAL:HG22	1:9:A:ILE:HG12	5	0.21
(1,728)	1:5:A:VAL:HG23	1:9:A:ILE:HG12	5	0.21
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	3	0.21
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	3	0.21
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	3	0.21
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	7	0.21
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	7	0.21
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	7	0.21
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	8	0.21
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	8	0.21
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	8	0.21
(1,681)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	3	0.21
(1,681)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	6	0.21
(1,673)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	3	0.21
(1,673)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	4	0.21
(1,581)	1:17:A:PRO:HB3	1:18:A:SER:H	1	0.21
(1,559)	1:10:A:GLN:HB2	1:11:A:TRP:H	8	0.21
(1,548)	1:5:A:VAL:HA	1:6:A:ARG:H	1	0.21
(1,548)	1:5:A:VAL:HA	1:6:A:ARG:H	2	0.21
(1,548)	1:5:A:VAL:HA	1:6:A:ARG:H	3	0.21
(1,548)	1:5:A:VAL:HA	1:6:A:ARG:H	5	0.21
(1,548)	1:5:A:VAL:HA	1:6:A:ARG:H	8	0.21
(1,534)	1:18:A:SER:HB3	1:19:A:SER:H	2	0.21
(1,534)	1:18:A:SER:HB3	1:19:A:SER:H	3	0.21
(1,534)	1:18:A:SER:HB3	1:19:A:SER:H	6	0.21
(1,534)	1:18:A:SER:HB3	1:19:A:SER:H	9	0.21
(1,493)	1:7:A:LEU:H	1:10:A:GLN:HB2	5	0.21
(1,493)	1:7:A:LEU:H	1:10:A:GLN:HB2	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.21
(1,402)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	4	0.21
(1,352)	1:8:A:TYR:HD1	1:9:A:ILE:HB	1	0.21
(1,352)	1:8:A:TYR:HD2	1:9:A:ILE:HB	1	0.21
(1,316)	1:1:A:GLU:HA	1:1:A:GLU:HG2	3	0.21
(1,316)	1:1:A:GLU:HA	1:1:A:GLU:HG2	4	0.21
(1,227)	1:18:A:SER:H	1:18:A:SER:HB3	2	0.21
(1,227)	1:18:A:SER:H	1:18:A:SER:HB3	3	0.21
(1,227)	1:18:A:SER:H	1:18:A:SER:HB3	4	0.21
(1,227)	1:18:A:SER:H	1:18:A:SER:HB3	10	0.21
(1,185)	1:13:A:LYS:HA	1:14:A:ASP:H	6	0.21
(1,161)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.21
(3,79)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	5	0.2
(3,79)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	5	0.2
(3,65)	1:5:A:VAL:HA	1:6:A:ARG:H	6	0.2
(3,65)	1:5:A:VAL:HA	1:6:A:ARG:H	7	0.2
(3,65)	1:5:A:VAL:HA	1:6:A:ARG:H	9	0.2
(3,65)	1:5:A:VAL:HA	1:6:A:ARG:H	10	0.2
(3,56)	1:7:A:LEU:H	1:10:A:GLN:HB2	7	0.2
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.2
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.2
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.2
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.2
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.2
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.2
(3,24)	1:13:A:LYS:HA	1:14:A:ASP:H	4	0.2
(3,21)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.2
(3,21)	1:12:A:LEU:H	1:12:A:LEU:HB3	5	0.2
(3,21)	1:12:A:LEU:H	1:12:A:LEU:HB3	7	0.2
(3,21)	1:12:A:LEU:H	1:12:A:LEU:HB3	8	0.2
(3,21)	1:12:A:LEU:H	1:12:A:LEU:HB3	9	0.2
(3,21)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.2
(2,665)	1:6:A:ARG:HB3	1:7:A:LEU:H	5	0.2
(2,665)	1:6:A:ARG:HB3	1:7:A:LEU:H	6	0.2
(2,665)	1:6:A:ARG:HB3	1:7:A:LEU:H	7	0.2
(2,647)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	4	0.2
(2,647)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	4	0.2
(2,647)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	4	0.2
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	10	0.2
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	10	0.2
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	10	0.2
(2,599)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,558)	1:22:A:PRO:HA	1:23:A:PRO:HG2	4	0.2
(2,520)	1:2:A:GLU:HA	1:5:A:VAL:H	9	0.2
(2,514)	1:24:A:PRO:HD3	1:25:A:SER:H	6	0.2
(2,382)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	1	0.2
(2,362)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	5	0.2
(2,362)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	7	0.2
(2,316)	1:8:A:TYR:HD1	1:9:A:ILE:HB	4	0.2
(2,316)	1:8:A:TYR:HD2	1:9:A:ILE:HB	4	0.2
(2,316)	1:8:A:TYR:HD1	1:9:A:ILE:HB	10	0.2
(2,316)	1:8:A:TYR:HD2	1:9:A:ILE:HB	10	0.2
(1,744)	1:6:A:ARG:HB3	1:7:A:LEU:H	5	0.2
(1,744)	1:6:A:ARG:HB3	1:7:A:LEU:H	6	0.2
(1,744)	1:6:A:ARG:HB3	1:7:A:LEU:H	7	0.2
(1,742)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	5	0.2
(1,742)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	5	0.2
(1,723)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	4	0.2
(1,723)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	4	0.2
(1,723)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	4	0.2
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	10	0.2
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	10	0.2
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	10	0.2
(1,673)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	6	0.2
(1,630)	1:22:A:PRO:HA	1:23:A:PRO:HG2	4	0.2
(1,591)	1:2:A:GLU:HA	1:5:A:VAL:H	9	0.2
(1,585)	1:24:A:PRO:HD3	1:25:A:SER:H	6	0.2
(1,548)	1:5:A:VAL:HA	1:6:A:ARG:H	6	0.2
(1,548)	1:5:A:VAL:HA	1:6:A:ARG:H	7	0.2
(1,548)	1:5:A:VAL:HA	1:6:A:ARG:H	9	0.2
(1,548)	1:5:A:VAL:HA	1:6:A:ARG:H	10	0.2
(1,493)	1:7:A:LEU:H	1:10:A:GLN:HB2	7	0.2
(1,426)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	1	0.2
(1,405)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	5	0.2
(1,405)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	7	0.2
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.2
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.2
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.2
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.2
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.2
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.2
(1,352)	1:8:A:TYR:HD1	1:9:A:ILE:HB	4	0.2
(1,352)	1:8:A:TYR:HD2	1:9:A:ILE:HB	4	0.2
(1,352)	1:8:A:TYR:HD1	1:9:A:ILE:HB	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:8:A:TYR:HD2	1:9:A:ILE:HB	10	0.2
(1,185)	1:13:A:LYS:HA	1:14:A:ASP:H	4	0.2
(1,161)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.2
(1,161)	1:12:A:LEU:H	1:12:A:LEU:HB3	5	0.2
(1,161)	1:12:A:LEU:H	1:12:A:LEU:HB3	7	0.2
(1,161)	1:12:A:LEU:H	1:12:A:LEU:HB3	8	0.2
(1,161)	1:12:A:LEU:H	1:12:A:LEU:HB3	9	0.2
(1,161)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.2
(3,79)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	6	0.19
(3,79)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	6	0.19
(3,79)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	7	0.19
(3,79)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	7	0.19
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.19
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.19
(3,24)	1:13:A:LYS:HA	1:14:A:ASP:H	2	0.19
(3,24)	1:13:A:LYS:HA	1:14:A:ASP:H	3	0.19
(3,24)	1:13:A:LYS:HA	1:14:A:ASP:H	7	0.19
(3,24)	1:13:A:LYS:HA	1:14:A:ASP:H	8	0.19
(3,24)	1:13:A:LYS:HA	1:14:A:ASP:H	10	0.19
(3,21)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.19
(2,665)	1:6:A:ARG:HB3	1:7:A:LEU:H	1	0.19
(2,665)	1:6:A:ARG:HB3	1:7:A:LEU:H	8	0.19
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	1	0.19
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	1	0.19
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	1	0.19
(2,599)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	7	0.19
(2,599)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.19
(2,558)	1:22:A:PRO:HA	1:23:A:PRO:HG2	2	0.19
(2,558)	1:22:A:PRO:HA	1:23:A:PRO:HG2	3	0.19
(2,558)	1:22:A:PRO:HA	1:23:A:PRO:HG2	6	0.19
(2,558)	1:22:A:PRO:HA	1:23:A:PRO:HG2	8	0.19
(2,558)	1:22:A:PRO:HA	1:23:A:PRO:HG2	9	0.19
(2,501)	1:13:A:LYS:HG2	1:14:A:ASP:H	9	0.19
(2,470)	1:18:A:SER:HB3	1:19:A:SER:H	1	0.19
(2,470)	1:18:A:SER:HB3	1:19:A:SER:H	4	0.19
(2,391)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	3	0.19
(2,382)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	2	0.19
(2,382)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	3	0.19
(2,382)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	4	0.19
(2,382)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	5	0.19
(2,382)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	6	0.19
(2,382)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,382)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	8	0.19
(2,382)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	9	0.19
(2,382)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	10	0.19
(2,359)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	6	0.19
(2,359)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	7	0.19
(2,359)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	10	0.19
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	5	0.19
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	5	0.19
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	5	0.19
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	5	0.19
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	5	0.19
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	5	0.19
(1,744)	1:6:A:ARG:HB3	1:7:A:LEU:H	1	0.19
(1,744)	1:6:A:ARG:HB3	1:7:A:LEU:H	8	0.19
(1,742)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	6	0.19
(1,742)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	6	0.19
(1,742)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	7	0.19
(1,742)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	7	0.19
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	1	0.19
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	1	0.19
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	1	0.19
(1,673)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	7	0.19
(1,673)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.19
(1,630)	1:22:A:PRO:HA	1:23:A:PRO:HG2	2	0.19
(1,630)	1:22:A:PRO:HA	1:23:A:PRO:HG2	3	0.19
(1,630)	1:22:A:PRO:HA	1:23:A:PRO:HG2	6	0.19
(1,630)	1:22:A:PRO:HA	1:23:A:PRO:HG2	8	0.19
(1,630)	1:22:A:PRO:HA	1:23:A:PRO:HG2	9	0.19
(1,569)	1:13:A:LYS:HG2	1:14:A:ASP:H	9	0.19
(1,534)	1:18:A:SER:HB3	1:19:A:SER:H	1	0.19
(1,534)	1:18:A:SER:HB3	1:19:A:SER:H	4	0.19
(1,435)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	3	0.19
(1,426)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	2	0.19
(1,426)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	3	0.19
(1,426)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	4	0.19
(1,426)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	5	0.19
(1,426)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	6	0.19
(1,426)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	7	0.19
(1,426)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	8	0.19
(1,426)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	9	0.19
(1,426)	1:11:A:TRP:HB3	1:11:A:TRP:HZ3	10	0.19
(1,402)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,402)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	7	0.19
(1,402)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	10	0.19
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.19
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.19
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	5	0.19
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	5	0.19
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	5	0.19
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	5	0.19
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	5	0.19
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	5	0.19
(1,185)	1:13:A:LYS:HA	1:14:A:ASP:H	2	0.19
(1,185)	1:13:A:LYS:HA	1:14:A:ASP:H	3	0.19
(1,185)	1:13:A:LYS:HA	1:14:A:ASP:H	7	0.19
(1,185)	1:13:A:LYS:HA	1:14:A:ASP:H	8	0.19
(1,185)	1:13:A:LYS:HA	1:14:A:ASP:H	10	0.19
(1,161)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.19
(3,79)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	2	0.18
(3,79)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	2	0.18
(3,67)	1:10:A:GLN:HB2	1:11:A:TRP:H	1	0.18
(3,67)	1:10:A:GLN:HB2	1:11:A:TRP:H	2	0.18
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.18
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.18
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.18
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.18
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.18
(3,40)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.18
(3,24)	1:13:A:LYS:HA	1:14:A:ASP:H	1	0.18
(3,24)	1:13:A:LYS:HA	1:14:A:ASP:H	5	0.18
(2,665)	1:6:A:ARG:HB3	1:7:A:LEU:H	2	0.18
(2,665)	1:6:A:ARG:HB3	1:7:A:LEU:H	3	0.18
(2,665)	1:6:A:ARG:HB3	1:7:A:LEU:H	4	0.18
(2,665)	1:6:A:ARG:HB3	1:7:A:LEU:H	10	0.18
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	2	0.18
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	2	0.18
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	2	0.18
(2,607)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	9	0.18
(2,599)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	5	0.18
(2,595)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	1	0.18
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	1	0.18
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	1	0.18
(2,595)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	2	0.18
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	2	0.18
(2,501)	1:13:A:LYS:HG2	1:14:A:ASP:H	1	0.18
(2,501)	1:13:A:LYS:HG2	1:14:A:ASP:H	5	0.18
(2,501)	1:13:A:LYS:HG2	1:14:A:ASP:H	8	0.18
(2,498)	1:13:A:LYS:HD2	1:14:A:ASP:H	3	0.18
(2,498)	1:13:A:LYS:HD3	1:14:A:ASP:H	3	0.18
(2,414)	1:2:A:GLU:HA	1:2:A:GLU:HB3	3	0.18
(2,414)	1:2:A:GLU:HA	1:2:A:GLU:HB3	5	0.18
(2,414)	1:2:A:GLU:HA	1:2:A:GLU:HB3	6	0.18
(2,414)	1:2:A:GLU:HA	1:2:A:GLU:HB3	7	0.18
(2,391)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	4	0.18
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	8	0.18
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	8	0.18
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	8	0.18
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	8	0.18
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	8	0.18
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	8	0.18
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE1	5	0.18
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE2	5	0.18
(1,744)	1:6:A:ARG:HB3	1:7:A:LEU:H	2	0.18
(1,744)	1:6:A:ARG:HB3	1:7:A:LEU:H	3	0.18
(1,744)	1:6:A:ARG:HB3	1:7:A:LEU:H	4	0.18
(1,744)	1:6:A:ARG:HB3	1:7:A:LEU:H	10	0.18
(1,742)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	2	0.18
(1,742)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	2	0.18
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	2	0.18
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	2	0.18
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	2	0.18
(1,681)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	9	0.18
(1,673)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	5	0.18
(1,669)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	1	0.18
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	1	0.18
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	1	0.18
(1,669)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	2	0.18
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	2	0.18
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	2	0.18
(1,569)	1:13:A:LYS:HG2	1:14:A:ASP:H	1	0.18
(1,569)	1:13:A:LYS:HG2	1:14:A:ASP:H	5	0.18
(1,569)	1:13:A:LYS:HG2	1:14:A:ASP:H	8	0.18
(1,566)	1:13:A:LYS:HD2	1:14:A:ASP:H	3	0.18
(1,566)	1:13:A:LYS:HD3	1:14:A:ASP:H	3	0.18
(1,559)	1:10:A:GLN:HB2	1:11:A:TRP:H	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:10:A:GLN:HB2	1:11:A:TRP:H	2	0.18
(1,466)	1:2:A:GLU:HA	1:2:A:GLU:HB3	3	0.18
(1,466)	1:2:A:GLU:HA	1:2:A:GLU:HB3	5	0.18
(1,466)	1:2:A:GLU:HA	1:2:A:GLU:HB3	6	0.18
(1,466)	1:2:A:GLU:HA	1:2:A:GLU:HB3	7	0.18
(1,435)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	4	0.18
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.18
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.18
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.18
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.18
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.18
(1,358)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.18
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	8	0.18
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	8	0.18
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	8	0.18
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	8	0.18
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	8	0.18
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	8	0.18
(1,185)	1:13:A:LYS:HA	1:14:A:ASP:H	1	0.18
(1,185)	1:13:A:LYS:HA	1:14:A:ASP:H	5	0.18
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE1	5	0.18
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE2	5	0.18
(3,79)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	3	0.17
(3,79)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	3	0.17
(3,79)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	8	0.17
(3,79)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	8	0.17
(3,79)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	9	0.17
(3,79)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	9	0.17
(3,67)	1:10:A:GLN:HB2	1:11:A:TRP:H	4	0.17
(3,67)	1:10:A:GLN:HB2	1:11:A:TRP:H	10	0.17
(3,24)	1:13:A:LYS:HA	1:14:A:ASP:H	9	0.17
(2,595)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	5	0.17
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	5	0.17
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	5	0.17
(2,565)	1:2:A:GLU:HA	1:3:A:GLU:HB2	6	0.17
(2,510)	1:17:A:PRO:HB3	1:18:A:SER:H	2	0.17
(2,508)	1:24:A:PRO:HG2	1:25:A:SER:H	7	0.17
(2,501)	1:13:A:LYS:HG2	1:14:A:ASP:H	3	0.17
(2,501)	1:13:A:LYS:HG2	1:14:A:ASP:H	4	0.17
(2,501)	1:13:A:LYS:HG2	1:14:A:ASP:H	6	0.17
(2,501)	1:13:A:LYS:HG2	1:14:A:ASP:H	7	0.17
(2,501)	1:13:A:LYS:HG2	1:14:A:ASP:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,470)	1:18:A:SER:HB3	1:19:A:SER:H	10	0.17
(2,414)	1:2:A:GLU:HA	1:2:A:GLU:HB3	2	0.17
(2,414)	1:2:A:GLU:HA	1:2:A:GLU:HB3	10	0.17
(2,391)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	1	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	2	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	2	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	2	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	2	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	2	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	2	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	7	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	7	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	7	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	7	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	7	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	7	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	9	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	9	0.17
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	9	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	9	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	9	0.17
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	9	0.17
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE1	7	0.17
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE2	7	0.17
(1,742)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	3	0.17
(1,742)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	3	0.17
(1,742)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	8	0.17
(1,742)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	8	0.17
(1,742)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	9	0.17
(1,742)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	9	0.17
(1,669)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	5	0.17
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	5	0.17
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	5	0.17
(1,637)	1:2:A:GLU:HA	1:3:A:GLU:HB2	6	0.17
(1,581)	1:17:A:PRO:HB3	1:18:A:SER:H	2	0.17
(1,578)	1:24:A:PRO:HG2	1:25:A:SER:H	7	0.17
(1,569)	1:13:A:LYS:HG2	1:14:A:ASP:H	3	0.17
(1,569)	1:13:A:LYS:HG2	1:14:A:ASP:H	4	0.17
(1,569)	1:13:A:LYS:HG2	1:14:A:ASP:H	6	0.17
(1,569)	1:13:A:LYS:HG2	1:14:A:ASP:H	7	0.17
(1,569)	1:13:A:LYS:HG2	1:14:A:ASP:H	10	0.17
(1,559)	1:10:A:GLN:HB2	1:11:A:TRP:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:10:A:GLN:HB2	1:11:A:TRP:H	10	0.17
(1,534)	1:18:A:SER:HB3	1:19:A:SER:H	10	0.17
(1,466)	1:2:A:GLU:HA	1:2:A:GLU:HB3	2	0.17
(1,466)	1:2:A:GLU:HA	1:2:A:GLU:HB3	10	0.17
(1,435)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	1	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	2	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	2	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	2	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	2	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	2	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	2	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	7	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	7	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	7	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	7	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	7	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	7	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	9	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	9	0.17
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	9	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	9	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	9	0.17
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	9	0.17
(1,185)	1:13:A:LYS:HA	1:14:A:ASP:H	9	0.17
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE1	7	0.17
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE2	7	0.17
(3,67)	1:10:A:GLN:HB2	1:11:A:TRP:H	3	0.16
(3,67)	1:10:A:GLN:HB2	1:11:A:TRP:H	9	0.16
(3,53)	1:4:A:ALA:HA	1:7:A:LEU:H	5	0.16
(3,53)	1:4:A:ALA:HA	1:7:A:LEU:H	6	0.16
(2,656)	1:6:A:ARG:HG3	1:7:A:LEU:HD11	4	0.16
(2,656)	1:6:A:ARG:HG3	1:7:A:LEU:HD12	4	0.16
(2,656)	1:6:A:ARG:HG3	1:7:A:LEU:HD13	4	0.16
(2,623)	1:3:A:GLU:HG2	1:4:A:ALA:HB1	4	0.16
(2,623)	1:3:A:GLU:HG2	1:4:A:ALA:HB2	4	0.16
(2,623)	1:3:A:GLU:HG2	1:4:A:ALA:HB3	4	0.16
(2,615)	1:3:A:GLU:HG2	1:7:A:LEU:HG	5	0.16
(2,615)	1:3:A:GLU:HG2	1:7:A:LEU:HG	6	0.16
(2,615)	1:3:A:GLU:HG2	1:7:A:LEU:HG	9	0.16
(2,595)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	7	0.16
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	7	0.16
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,595)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	10	0.16
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	10	0.16
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	10	0.16
(2,508)	1:24:A:PRO:HG2	1:25:A:SER:H	10	0.16
(2,501)	1:13:A:LYS:HG2	1:14:A:ASP:H	2	0.16
(2,473)	1:7:A:LEU:HA	1:8:A:TYR:H	4	0.16
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD11	2	0.16
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD12	2	0.16
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD13	2	0.16
(2,414)	1:2:A:GLU:HA	1:2:A:GLU:HB3	8	0.16
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	6	0.16
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	6	0.16
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	6	0.16
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	6	0.16
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	6	0.16
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	6	0.16
(2,209)	1:21:A:ARG:H	1:21:A:ARG:HD3	2	0.16
(2,206)	1:20:A:GLY:H	1:20:A:GLY:HA3	4	0.16
(2,206)	1:20:A:GLY:H	1:20:A:GLY:HA3	6	0.16
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE1	2	0.16
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE2	2	0.16
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE1	3	0.16
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE2	3	0.16
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE1	6	0.16
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE2	6	0.16
(1,734)	1:6:A:ARG:HG3	1:7:A:LEU:HD11	4	0.16
(1,734)	1:6:A:ARG:HG3	1:7:A:LEU:HD12	4	0.16
(1,734)	1:6:A:ARG:HG3	1:7:A:LEU:HD13	4	0.16
(1,697)	1:3:A:GLU:HG2	1:4:A:ALA:HB1	4	0.16
(1,697)	1:3:A:GLU:HG2	1:4:A:ALA:HB2	4	0.16
(1,697)	1:3:A:GLU:HG2	1:4:A:ALA:HB3	4	0.16
(1,689)	1:3:A:GLU:HG2	1:7:A:LEU:HG	5	0.16
(1,689)	1:3:A:GLU:HG2	1:7:A:LEU:HG	6	0.16
(1,689)	1:3:A:GLU:HG2	1:7:A:LEU:HG	9	0.16
(1,669)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	7	0.16
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	7	0.16
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	7	0.16
(1,669)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	10	0.16
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	10	0.16
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	10	0.16
(1,578)	1:24:A:PRO:HG2	1:25:A:SER:H	10	0.16
(1,569)	1:13:A:LYS:HG2	1:14:A:ASP:H	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:10:A:GLN:HB2	1:11:A:TRP:H	3	0.16
(1,559)	1:10:A:GLN:HB2	1:11:A:TRP:H	9	0.16
(1,537)	1:7:A:LEU:HA	1:8:A:TYR:H	4	0.16
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD11	2	0.16
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD12	2	0.16
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD13	2	0.16
(1,475)	1:4:A:ALA:HA	1:7:A:LEU:H	5	0.16
(1,475)	1:4:A:ALA:HA	1:7:A:LEU:H	6	0.16
(1,466)	1:2:A:GLU:HA	1:2:A:GLU:HB3	8	0.16
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	6	0.16
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	6	0.16
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	6	0.16
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	6	0.16
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	6	0.16
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	6	0.16
(1,234)	1:21:A:ARG:H	1:21:A:ARG:HD3	2	0.16
(1,231)	1:20:A:GLY:H	1:20:A:GLY:HA3	4	0.16
(1,231)	1:20:A:GLY:H	1:20:A:GLY:HA3	6	0.16
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE1	2	0.16
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE2	2	0.16
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE1	3	0.16
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE2	3	0.16
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE1	6	0.16
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE2	6	0.16
(3,67)	1:10:A:GLN:HB2	1:11:A:TRP:H	6	0.15
(3,67)	1:10:A:GLN:HB2	1:11:A:TRP:H	7	0.15
(3,53)	1:4:A:ALA:HA	1:7:A:LEU:H	1	0.15
(3,53)	1:4:A:ALA:HA	1:7:A:LEU:H	8	0.15
(2,665)	1:6:A:ARG:HB3	1:7:A:LEU:H	9	0.15
(2,615)	1:3:A:GLU:HG2	1:7:A:LEU:HG	1	0.15
(2,615)	1:3:A:GLU:HG2	1:7:A:LEU:HG	2	0.15
(2,615)	1:3:A:GLU:HG2	1:7:A:LEU:HG	10	0.15
(2,530)	1:2:A:GLU:HB2	1:5:A:VAL:H	1	0.15
(2,514)	1:24:A:PRO:HD3	1:25:A:SER:H	10	0.15
(2,508)	1:24:A:PRO:HG2	1:25:A:SER:H	6	0.15
(2,498)	1:13:A:LYS:HD2	1:14:A:ASP:H	5	0.15
(2,498)	1:13:A:LYS:HD3	1:14:A:ASP:H	5	0.15
(2,473)	1:7:A:LEU:HA	1:8:A:TYR:H	3	0.15
(2,473)	1:7:A:LEU:HA	1:8:A:TYR:H	5	0.15
(2,473)	1:7:A:LEU:HA	1:8:A:TYR:H	6	0.15
(2,473)	1:7:A:LEU:HA	1:8:A:TYR:H	7	0.15
(2,473)	1:7:A:LEU:HA	1:8:A:TYR:H	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,473)	1:7:A:LEU:HA	1:8:A:TYR:H	9	0.15
(2,473)	1:7:A:LEU:HA	1:8:A:TYR:H	10	0.15
(2,432)	1:3:A:GLU:HG2	1:4:A:ALA:H	4	0.15
(2,414)	1:2:A:GLU:HA	1:2:A:GLU:HB3	1	0.15
(2,360)	1:14:A:ASP:HB2	1:21:A:ARG:HH11	8	0.15
(2,360)	1:14:A:ASP:HB2	1:21:A:ARG:HH12	8	0.15
(2,344)	1:11:A:TRP:HD1	1:23:A:PRO:HA	5	0.15
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	3	0.15
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	3	0.15
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	3	0.15
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	3	0.15
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	3	0.15
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	3	0.15
(2,206)	1:20:A:GLY:H	1:20:A:GLY:HA3	1	0.15
(2,206)	1:20:A:GLY:H	1:20:A:GLY:HA3	2	0.15
(2,206)	1:20:A:GLY:H	1:20:A:GLY:HA3	3	0.15
(2,206)	1:20:A:GLY:H	1:20:A:GLY:HA3	5	0.15
(2,206)	1:20:A:GLY:H	1:20:A:GLY:HA3	7	0.15
(2,206)	1:20:A:GLY:H	1:20:A:GLY:HA3	9	0.15
(2,206)	1:20:A:GLY:H	1:20:A:GLY:HA3	10	0.15
(1,744)	1:6:A:ARG:HB3	1:7:A:LEU:H	9	0.15
(1,689)	1:3:A:GLU:HG2	1:7:A:LEU:HG	1	0.15
(1,689)	1:3:A:GLU:HG2	1:7:A:LEU:HG	2	0.15
(1,689)	1:3:A:GLU:HG2	1:7:A:LEU:HG	10	0.15
(1,602)	1:2:A:GLU:HB2	1:5:A:VAL:H	1	0.15
(1,585)	1:24:A:PRO:HD3	1:25:A:SER:H	10	0.15
(1,578)	1:24:A:PRO:HG2	1:25:A:SER:H	6	0.15
(1,566)	1:13:A:LYS:HD2	1:14:A:ASP:H	5	0.15
(1,566)	1:13:A:LYS:HD3	1:14:A:ASP:H	5	0.15
(1,559)	1:10:A:GLN:HB2	1:11:A:TRP:H	6	0.15
(1,559)	1:10:A:GLN:HB2	1:11:A:TRP:H	7	0.15
(1,537)	1:7:A:LEU:HA	1:8:A:TYR:H	3	0.15
(1,537)	1:7:A:LEU:HA	1:8:A:TYR:H	5	0.15
(1,537)	1:7:A:LEU:HA	1:8:A:TYR:H	6	0.15
(1,537)	1:7:A:LEU:HA	1:8:A:TYR:H	7	0.15
(1,537)	1:7:A:LEU:HA	1:8:A:TYR:H	8	0.15
(1,537)	1:7:A:LEU:HA	1:8:A:TYR:H	9	0.15
(1,537)	1:7:A:LEU:HA	1:8:A:TYR:H	10	0.15
(1,487)	1:3:A:GLU:HG2	1:4:A:ALA:H	4	0.15
(1,475)	1:4:A:ALA:HA	1:7:A:LEU:H	1	0.15
(1,475)	1:4:A:ALA:HA	1:7:A:LEU:H	8	0.15
(1,466)	1:2:A:GLU:HA	1:2:A:GLU:HB3	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,403)	1:14:A:ASP:HB2	1:21:A:ARG:HH11	8	0.15
(1,403)	1:14:A:ASP:HB2	1:21:A:ARG:HH12	8	0.15
(1,385)	1:11:A:TRP:HD1	1:23:A:PRO:HA	5	0.15
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	3	0.15
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	3	0.15
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	3	0.15
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	3	0.15
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	3	0.15
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	3	0.15
(1,231)	1:20:A:GLY:H	1:20:A:GLY:HA3	1	0.15
(1,231)	1:20:A:GLY:H	1:20:A:GLY:HA3	2	0.15
(1,231)	1:20:A:GLY:H	1:20:A:GLY:HA3	3	0.15
(1,231)	1:20:A:GLY:H	1:20:A:GLY:HA3	5	0.15
(1,231)	1:20:A:GLY:H	1:20:A:GLY:HA3	7	0.15
(1,231)	1:20:A:GLY:H	1:20:A:GLY:HA3	9	0.15
(1,231)	1:20:A:GLY:H	1:20:A:GLY:HA3	10	0.15
(3,67)	1:10:A:GLN:HB2	1:11:A:TRP:H	5	0.14
(3,53)	1:4:A:ALA:HA	1:7:A:LEU:H	2	0.14
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	5	0.14
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	5	0.14
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	5	0.14
(2,618)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	2	0.14
(2,615)	1:3:A:GLU:HG2	1:7:A:LEU:HG	8	0.14
(2,600)	1:14:A:ASP:HB2	1:19:A:SER:HB3	3	0.14
(2,600)	1:14:A:ASP:HB2	1:19:A:SER:HB3	4	0.14
(2,600)	1:14:A:ASP:HB2	1:19:A:SER:HB3	6	0.14
(2,530)	1:2:A:GLU:HB2	1:5:A:VAL:H	8	0.14
(2,498)	1:13:A:LYS:HD2	1:14:A:ASP:H	1	0.14
(2,498)	1:13:A:LYS:HD3	1:14:A:ASP:H	1	0.14
(2,498)	1:13:A:LYS:HD2	1:14:A:ASP:H	8	0.14
(2,498)	1:13:A:LYS:HD3	1:14:A:ASP:H	8	0.14
(2,473)	1:7:A:LEU:HA	1:8:A:TYR:H	1	0.14
(2,473)	1:7:A:LEU:HA	1:8:A:TYR:H	2	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD11	5	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD12	5	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD13	5	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD11	6	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD12	6	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD13	6	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD11	8	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD12	8	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD13	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD11	10	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD12	10	0.14
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD13	10	0.14
(2,344)	1:11:A:TRP:HD1	1:23:A:PRO:HA	1	0.14
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	2	0.14
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	4	0.14
(2,206)	1:20:A:GLY:H	1:20:A:GLY:HA3	8	0.14
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE1	8	0.14
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE2	8	0.14
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE1	9	0.14
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE2	9	0.14
(2,32)	1:6:A:ARG:HA	1:6:A:ARG:HG3	4	0.14
(2,32)	1:6:A:ARG:HA	1:6:A:ARG:HG3	5	0.14
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	5	0.14
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	5	0.14
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	5	0.14
(1,692)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	2	0.14
(1,689)	1:3:A:GLU:HG2	1:7:A:LEU:HG	8	0.14
(1,674)	1:14:A:ASP:HB2	1:19:A:SER:HB3	3	0.14
(1,674)	1:14:A:ASP:HB2	1:19:A:SER:HB3	4	0.14
(1,674)	1:14:A:ASP:HB2	1:19:A:SER:HB3	6	0.14
(1,602)	1:2:A:GLU:HB2	1:5:A:VAL:H	8	0.14
(1,566)	1:13:A:LYS:HD2	1:14:A:ASP:H	1	0.14
(1,566)	1:13:A:LYS:HD3	1:14:A:ASP:H	1	0.14
(1,566)	1:13:A:LYS:HD2	1:14:A:ASP:H	8	0.14
(1,566)	1:13:A:LYS:HD3	1:14:A:ASP:H	8	0.14
(1,559)	1:10:A:GLN:HB2	1:11:A:TRP:H	5	0.14
(1,537)	1:7:A:LEU:HA	1:8:A:TYR:H	1	0.14
(1,537)	1:7:A:LEU:HA	1:8:A:TYR:H	2	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD11	5	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD12	5	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD13	5	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD11	6	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD12	6	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD13	6	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD11	8	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD12	8	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD13	8	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD11	10	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD12	10	0.14
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD13	10	0.14
(1,475)	1:4:A:ALA:HA	1:7:A:LEU:H	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:11:A:TRP:HD1	1:23:A:PRO:HA	1	0.14
(1,360)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	2	0.14
(1,360)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	4	0.14
(1,231)	1:20:A:GLY:H	1:20:A:GLY:HA3	8	0.14
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE1	8	0.14
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE2	8	0.14
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE1	9	0.14
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE2	9	0.14
(1,39)	1:6:A:ARG:HA	1:6:A:ARG:HG3	4	0.14
(1,39)	1:6:A:ARG:HA	1:6:A:ARG:HG3	5	0.14
(3,53)	1:4:A:ALA:HA	1:7:A:LEU:H	3	0.13
(3,53)	1:4:A:ALA:HA	1:7:A:LEU:H	10	0.13
(3,1)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	4	0.13
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	9	0.13
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	9	0.13
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	9	0.13
(2,618)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	4	0.13
(2,615)	1:3:A:GLU:HG2	1:7:A:LEU:HG	3	0.13
(2,595)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	3	0.13
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	3	0.13
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	3	0.13
(2,595)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	4	0.13
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	4	0.13
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	4	0.13
(2,595)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	6	0.13
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	6	0.13
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	6	0.13
(2,595)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	8	0.13
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	8	0.13
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	8	0.13
(2,595)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	9	0.13
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	9	0.13
(2,595)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	9	0.13
(2,565)	1:2:A:GLU:HA	1:3:A:GLU:HB2	4	0.13
(2,558)	1:22:A:PRO:HA	1:23:A:PRO:HG2	5	0.13
(2,558)	1:22:A:PRO:HA	1:23:A:PRO:HG2	10	0.13
(2,530)	1:2:A:GLU:HB2	1:5:A:VAL:H	5	0.13
(2,509)	1:24:A:PRO:HB2	1:25:A:SER:H	1	0.13
(2,508)	1:24:A:PRO:HG2	1:25:A:SER:H	4	0.13
(2,507)	1:23:A:PRO:HB3	1:25:A:SER:H	5	0.13
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD11	6	0.13
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD12	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD13	6	0.13
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD11	7	0.13
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD12	7	0.13
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD13	7	0.13
(2,498)	1:13:A:LYS:HD2	1:14:A:ASP:H	2	0.13
(2,498)	1:13:A:LYS:HD3	1:14:A:ASP:H	2	0.13
(2,498)	1:13:A:LYS:HD2	1:14:A:ASP:H	4	0.13
(2,498)	1:13:A:LYS:HD3	1:14:A:ASP:H	4	0.13
(2,498)	1:13:A:LYS:HD2	1:14:A:ASP:H	10	0.13
(2,498)	1:13:A:LYS:HD3	1:14:A:ASP:H	10	0.13
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD11	1	0.13
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD12	1	0.13
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD13	1	0.13
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD11	3	0.13
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD12	3	0.13
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD13	3	0.13
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD11	7	0.13
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD12	7	0.13
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD13	7	0.13
(2,414)	1:2:A:GLU:HA	1:2:A:GLU:HB3	4	0.13
(2,360)	1:14:A:ASP:HB2	1:21:A:ARG:HH11	5	0.13
(2,360)	1:14:A:ASP:HB2	1:21:A:ARG:HH12	5	0.13
(2,349)	1:11:A:TRP:HH2	1:22:A:PRO:HA	5	0.13
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	6	0.13
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	8	0.13
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	9	0.13
(2,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	8	0.13
(2,32)	1:6:A:ARG:HA	1:6:A:ARG:HG3	1	0.13
(2,32)	1:6:A:ARG:HA	1:6:A:ARG:HG3	2	0.13
(2,32)	1:6:A:ARG:HA	1:6:A:ARG:HG3	3	0.13
(2,32)	1:6:A:ARG:HA	1:6:A:ARG:HG3	8	0.13
(2,32)	1:6:A:ARG:HA	1:6:A:ARG:HG3	10	0.13
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	9	0.13
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	9	0.13
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	9	0.13
(1,692)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	4	0.13
(1,689)	1:3:A:GLU:HG2	1:7:A:LEU:HG	3	0.13
(1,669)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	3	0.13
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	3	0.13
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	3	0.13
(1,669)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	4	0.13
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	4	0.13
(1,669)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	6	0.13
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	6	0.13
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	6	0.13
(1,669)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	8	0.13
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	8	0.13
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	8	0.13
(1,669)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	9	0.13
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	9	0.13
(1,669)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	9	0.13
(1,637)	1:2:A:GLU:HA	1:3:A:GLU:HB2	4	0.13
(1,630)	1:22:A:PRO:HA	1:23:A:PRO:HG2	5	0.13
(1,630)	1:22:A:PRO:HA	1:23:A:PRO:HG2	10	0.13
(1,602)	1:2:A:GLU:HB2	1:5:A:VAL:H	5	0.13
(1,580)	1:24:A:PRO:HB2	1:25:A:SER:H	1	0.13
(1,578)	1:24:A:PRO:HG2	1:25:A:SER:H	4	0.13
(1,577)	1:23:A:PRO:HB3	1:25:A:SER:H	5	0.13
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD11	6	0.13
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD12	6	0.13
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD13	6	0.13
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD11	7	0.13
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD12	7	0.13
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD13	7	0.13
(1,566)	1:13:A:LYS:HD2	1:14:A:ASP:H	2	0.13
(1,566)	1:13:A:LYS:HD3	1:14:A:ASP:H	2	0.13
(1,566)	1:13:A:LYS:HD2	1:14:A:ASP:H	4	0.13
(1,566)	1:13:A:LYS:HD3	1:14:A:ASP:H	4	0.13
(1,566)	1:13:A:LYS:HD2	1:14:A:ASP:H	10	0.13
(1,566)	1:13:A:LYS:HD3	1:14:A:ASP:H	10	0.13
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD11	1	0.13
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD12	1	0.13
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD13	1	0.13
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD11	3	0.13
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD12	3	0.13
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD13	3	0.13
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD11	7	0.13
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD12	7	0.13
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD13	7	0.13
(1,475)	1:4:A:ALA:HA	1:7:A:LEU:H	3	0.13
(1,475)	1:4:A:ALA:HA	1:7:A:LEU:H	10	0.13
(1,466)	1:2:A:GLU:HA	1:2:A:GLU:HB3	4	0.13
(1,403)	1:14:A:ASP:HB2	1:21:A:ARG:HH11	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,403)	1:14:A:ASP:HB2	1:21:A:ARG:HH12	5	0.13
(1,391)	1:11:A:TRP:HH2	1:22:A:PRO:HA	5	0.13
(1,360)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	6	0.13
(1,360)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	8	0.13
(1,360)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	9	0.13
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	8	0.13
(1,39)	1:6:A:ARG:HA	1:6:A:ARG:HG3	1	0.13
(1,39)	1:6:A:ARG:HA	1:6:A:ARG:HG3	2	0.13
(1,39)	1:6:A:ARG:HA	1:6:A:ARG:HG3	3	0.13
(1,39)	1:6:A:ARG:HA	1:6:A:ARG:HG3	8	0.13
(1,39)	1:6:A:ARG:HA	1:6:A:ARG:HG3	10	0.13
(1,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	4	0.13
(3,53)	1:4:A:ALA:HA	1:7:A:LEU:H	4	0.12
(3,28)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	3	0.12
(3,28)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	4	0.12
(3,28)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	6	0.12
(3,28)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	8	0.12
(3,28)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	9	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	1	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	1	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	1	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	1	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	1	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	1	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	1	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	1	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	1	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	4	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	4	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	4	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	4	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	4	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	4	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	4	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	4	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	4	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	7	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	7	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	7	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	7	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	7	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	7	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	7	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	7	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	8	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	8	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	8	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	8	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	8	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	8	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	8	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	8	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	8	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.12
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.12
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.12
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.12
(2,619)	1:2:A:GLU:HB3	1:6:A:ARG:HG3	6	0.12
(2,618)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	5	0.12
(2,618)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	6	0.12
(2,587)	1:1:A:GLU:HA	1:2:A:GLU:HB3	4	0.12
(2,587)	1:1:A:GLU:HA	1:2:A:GLU:HB3	9	0.12
(2,565)	1:2:A:GLU:HA	1:3:A:GLU:HB2	1	0.12
(2,558)	1:22:A:PRO:HA	1:23:A:PRO:HG2	7	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD11	5	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD12	5	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD13	5	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD11	8	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD12	8	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD13	8	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD11	9	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD12	9	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD13	9	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD11	10	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD12	10	0.12
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD13	10	0.12
(2,498)	1:13:A:LYS:HD2	1:14:A:ASP:H	6	0.12
(2,498)	1:13:A:LYS:HD3	1:14:A:ASP:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,498)	1:13:A:LYS:HD2	1:14:A:ASP:H	7	0.12
(2,498)	1:13:A:LYS:HD3	1:14:A:ASP:H	7	0.12
(2,498)	1:13:A:LYS:HD2	1:14:A:ASP:H	9	0.12
(2,498)	1:13:A:LYS:HD3	1:14:A:ASP:H	9	0.12
(2,472)	1:19:A:SER:HA	1:21:A:ARG:H	2	0.12
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD11	4	0.12
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD12	4	0.12
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD13	4	0.12
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD11	9	0.12
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD12	9	0.12
(2,457)	1:8:A:TYR:H	1:9:A:ILE:HD13	9	0.12
(2,412)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	1	0.12
(2,412)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	2	0.12
(2,412)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	5	0.12
(2,412)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	7	0.12
(2,412)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	10	0.12
(2,349)	1:11:A:TRP:HH2	1:22:A:PRO:HA	1	0.12
(2,322)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	2	0.12
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	3	0.12
(2,312)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	1	0.12
(2,312)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	1	0.12
(2,312)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	1	0.12
(2,312)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	1	0.12
(2,312)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	1	0.12
(2,312)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	1	0.12
(2,184)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	2	0.12
(2,179)	1:17:A:PRO:HA	1:17:A:PRO:HB2	2	0.12
(2,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	1	0.12
(2,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	3	0.12
(2,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	4	0.12
(2,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	5	0.12
(2,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	6	0.12
(2,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	7	0.12
(2,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	9	0.12
(2,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	10	0.12
(2,32)	1:6:A:ARG:HA	1:6:A:ARG:HG3	6	0.12
(2,32)	1:6:A:ARG:HA	1:6:A:ARG:HG3	7	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	1	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	1	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	1	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	1	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	1	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	1	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	1	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	1	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	4	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	4	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	4	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	4	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	4	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	4	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	4	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	4	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	4	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	7	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	7	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	7	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	7	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	7	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	7	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	7	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	7	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	7	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	8	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	8	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	8	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	8	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	8	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	8	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	8	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	8	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	8	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.12
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.12
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.12
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.12
(1,693)	1:2:A:GLU:HB3	1:6:A:ARG:HG3	6	0.12
(1,692)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,692)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	6	0.12
(1,660)	1:1:A:GLU:HA	1:2:A:GLU:HB3	4	0.12
(1,660)	1:1:A:GLU:HA	1:2:A:GLU:HB3	9	0.12
(1,637)	1:2:A:GLU:HA	1:3:A:GLU:HB2	1	0.12
(1,630)	1:22:A:PRO:HA	1:23:A:PRO:HG2	7	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD11	5	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD12	5	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD13	5	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD11	8	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD12	8	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD13	8	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD11	9	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD12	9	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD13	9	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD11	10	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD12	10	0.12
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD13	10	0.12
(1,566)	1:13:A:LYS:HD2	1:14:A:ASP:H	6	0.12
(1,566)	1:13:A:LYS:HD3	1:14:A:ASP:H	6	0.12
(1,566)	1:13:A:LYS:HD2	1:14:A:ASP:H	7	0.12
(1,566)	1:13:A:LYS:HD3	1:14:A:ASP:H	7	0.12
(1,566)	1:13:A:LYS:HD2	1:14:A:ASP:H	9	0.12
(1,566)	1:13:A:LYS:HD3	1:14:A:ASP:H	9	0.12
(1,536)	1:19:A:SER:HA	1:21:A:ARG:H	2	0.12
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD11	4	0.12
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD12	4	0.12
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD13	4	0.12
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD11	9	0.12
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD12	9	0.12
(1,519)	1:8:A:TYR:H	1:9:A:ILE:HD13	9	0.12
(1,475)	1:4:A:ALA:HA	1:7:A:LEU:H	4	0.12
(1,463)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	1	0.12
(1,463)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	2	0.12
(1,463)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	5	0.12
(1,463)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	7	0.12
(1,463)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	10	0.12
(1,391)	1:11:A:TRP:HH2	1:22:A:PRO:HA	1	0.12
(1,362)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	2	0.12
(1,360)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	3	0.12
(1,347)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	1	0.12
(1,347)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	1	0.12
(1,347)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	1	0.12
(1,347)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	1	0.12
(1,347)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	1	0.12
(1,274)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	3	0.12
(1,274)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	4	0.12
(1,274)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	6	0.12
(1,274)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	8	0.12
(1,274)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	9	0.12
(1,208)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	2	0.12
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB2	2	0.12
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	1	0.12
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	3	0.12
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	4	0.12
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	5	0.12
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	6	0.12
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	7	0.12
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	9	0.12
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	10	0.12
(1,39)	1:6:A:ARG:HA	1:6:A:ARG:HG3	6	0.12
(1,39)	1:6:A:ARG:HA	1:6:A:ARG:HG3	7	0.12
(3,53)	1:4:A:ALA:HA	1:7:A:LEU:H	9	0.11
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	2	0.11
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	2	0.11
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	2	0.11
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	2	0.11
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	2	0.11
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	2	0.11
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	2	0.11
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	2	0.11
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	2	0.11
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	9	0.11
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	9	0.11
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	9	0.11
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	9	0.11
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	9	0.11
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	9	0.11
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	9	0.11
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	9	0.11
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	9	0.11
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	6	0.11
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	6	0.11
(2,646)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,619)	1:2:A:GLU:HB3	1:6:A:ARG:HG3	3	0.11
(2,618)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	7	0.11
(2,615)	1:3:A:GLU:HG2	1:7:A:LEU:HG	7	0.11
(2,600)	1:14:A:ASP:HB2	1:19:A:SER:HB3	10	0.11
(2,558)	1:22:A:PRO:HA	1:23:A:PRO:HG2	1	0.11
(2,530)	1:2:A:GLU:HB2	1:5:A:VAL:H	2	0.11
(2,530)	1:2:A:GLU:HB2	1:5:A:VAL:H	10	0.11
(2,509)	1:24:A:PRO:HB2	1:25:A:SER:H	2	0.11
(2,509)	1:24:A:PRO:HB2	1:25:A:SER:H	9	0.11
(2,508)	1:24:A:PRO:HG2	1:25:A:SER:H	3	0.11
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD11	1	0.11
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD12	1	0.11
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD13	1	0.11
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD11	3	0.11
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD12	3	0.11
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD13	3	0.11
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD11	4	0.11
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD12	4	0.11
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD13	4	0.11
(2,455)	1:9:A:ILE:HG21	1:13:A:LYS:H	3	0.11
(2,455)	1:9:A:ILE:HG22	1:13:A:LYS:H	3	0.11
(2,455)	1:9:A:ILE:HG23	1:13:A:LYS:H	3	0.11
(2,455)	1:9:A:ILE:HG21	1:13:A:LYS:H	5	0.11
(2,455)	1:9:A:ILE:HG22	1:13:A:LYS:H	5	0.11
(2,455)	1:9:A:ILE:HG23	1:13:A:LYS:H	5	0.11
(2,455)	1:9:A:ILE:HG21	1:13:A:LYS:H	6	0.11
(2,455)	1:9:A:ILE:HG22	1:13:A:LYS:H	6	0.11
(2,455)	1:9:A:ILE:HG23	1:13:A:LYS:H	6	0.11
(2,455)	1:9:A:ILE:HG21	1:13:A:LYS:H	7	0.11
(2,455)	1:9:A:ILE:HG22	1:13:A:LYS:H	7	0.11
(2,455)	1:9:A:ILE:HG23	1:13:A:LYS:H	7	0.11
(2,442)	1:5:A:VAL:HG21	1:7:A:LEU:H	4	0.11
(2,442)	1:5:A:VAL:HG22	1:7:A:LEU:H	4	0.11
(2,442)	1:5:A:VAL:HG23	1:7:A:LEU:H	4	0.11
(2,412)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	3	0.11
(2,412)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	4	0.11
(2,412)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	6	0.11
(2,412)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	8	0.11
(2,412)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	9	0.11
(2,391)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	5	0.11
(2,350)	1:11:A:TRP:HH2	1:17:A:PRO:HA	2	0.11
(2,350)	1:11:A:TRP:HH2	1:17:A:PRO:HA	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,349)	1:11:A:TRP:HH2	1:22:A:PRO:HA	7	0.11
(2,344)	1:11:A:TRP:HD1	1:23:A:PRO:HA	3	0.11
(2,344)	1:11:A:TRP:HD1	1:23:A:PRO:HA	4	0.11
(2,344)	1:11:A:TRP:HD1	1:23:A:PRO:HA	6	0.11
(2,344)	1:11:A:TRP:HD1	1:23:A:PRO:HA	7	0.11
(2,344)	1:11:A:TRP:HD1	1:23:A:PRO:HA	8	0.11
(2,336)	1:8:A:TYR:HA	1:11:A:TRP:HD1	1	0.11
(2,336)	1:8:A:TYR:HA	1:11:A:TRP:HD1	3	0.11
(2,336)	1:8:A:TYR:HA	1:11:A:TRP:HD1	6	0.11
(2,336)	1:8:A:TYR:HA	1:11:A:TRP:HD1	10	0.11
(2,322)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	3	0.11
(2,322)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	6	0.11
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	7	0.11
(2,320)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	10	0.11
(2,312)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	10	0.11
(2,312)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	10	0.11
(2,312)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	10	0.11
(2,312)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	10	0.11
(2,312)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	10	0.11
(2,312)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	10	0.11
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	10	0.11
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	10	0.11
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	10	0.11
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	10	0.11
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	10	0.11
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	10	0.11
(2,297)	1:5:A:VAL:HA	1:8:A:TYR:HE1	4	0.11
(2,297)	1:5:A:VAL:HA	1:8:A:TYR:HE2	4	0.11
(2,208)	1:21:A:ARG:H	1:21:A:ARG:HD2	10	0.11
(2,184)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	1	0.11
(2,184)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	3	0.11
(2,184)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	4	0.11
(2,184)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	5	0.11
(2,184)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	8	0.11
(2,179)	1:17:A:PRO:HA	1:17:A:PRO:HB2	1	0.11
(2,179)	1:17:A:PRO:HA	1:17:A:PRO:HB2	4	0.11
(2,179)	1:17:A:PRO:HA	1:17:A:PRO:HB2	8	0.11
(2,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	2	0.11
(2,69)	1:7:A:LEU:H	1:7:A:LEU:HB3	4	0.11
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	2	0.11
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	2	0.11
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	2	0.11
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	2	0.11
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	2	0.11
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	2	0.11
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	2	0.11
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	2	0.11
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	9	0.11
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	9	0.11
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	9	0.11
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	9	0.11
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	9	0.11
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	9	0.11
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	9	0.11
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	9	0.11
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	9	0.11
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD21	6	0.11
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD22	6	0.11
(1,722)	1:3:A:GLU:HG3	1:7:A:LEU:HD23	6	0.11
(1,693)	1:2:A:GLU:HB3	1:6:A:ARG:HG3	3	0.11
(1,692)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	7	0.11
(1,689)	1:3:A:GLU:HG2	1:7:A:LEU:HG	7	0.11
(1,674)	1:14:A:ASP:HB2	1:19:A:SER:HB3	10	0.11
(1,630)	1:22:A:PRO:HA	1:23:A:PRO:HG2	1	0.11
(1,602)	1:2:A:GLU:HB2	1:5:A:VAL:H	2	0.11
(1,602)	1:2:A:GLU:HB2	1:5:A:VAL:H	10	0.11
(1,580)	1:24:A:PRO:HB2	1:25:A:SER:H	2	0.11
(1,580)	1:24:A:PRO:HB2	1:25:A:SER:H	9	0.11
(1,578)	1:24:A:PRO:HG2	1:25:A:SER:H	3	0.11
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD11	1	0.11
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD12	1	0.11
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD13	1	0.11
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD11	3	0.11
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD12	3	0.11
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD13	3	0.11
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD11	4	0.11
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD12	4	0.11
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD13	4	0.11
(1,516)	1:9:A:ILE:HG21	1:13:A:LYS:H	3	0.11
(1,516)	1:9:A:ILE:HG22	1:13:A:LYS:H	3	0.11
(1,516)	1:9:A:ILE:HG23	1:13:A:LYS:H	3	0.11
(1,516)	1:9:A:ILE:HG21	1:13:A:LYS:H	5	0.11
(1,516)	1:9:A:ILE:HG22	1:13:A:LYS:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:9:A:ILE:HG23	1:13:A:LYS:H	5	0.11
(1,516)	1:9:A:ILE:HG21	1:13:A:LYS:H	6	0.11
(1,516)	1:9:A:ILE:HG22	1:13:A:LYS:H	6	0.11
(1,516)	1:9:A:ILE:HG23	1:13:A:LYS:H	6	0.11
(1,516)	1:9:A:ILE:HG21	1:13:A:LYS:H	7	0.11
(1,516)	1:9:A:ILE:HG22	1:13:A:LYS:H	7	0.11
(1,516)	1:9:A:ILE:HG23	1:13:A:LYS:H	7	0.11
(1,502)	1:5:A:VAL:HG21	1:7:A:LEU:H	4	0.11
(1,502)	1:5:A:VAL:HG22	1:7:A:LEU:H	4	0.11
(1,502)	1:5:A:VAL:HG23	1:7:A:LEU:H	4	0.11
(1,475)	1:4:A:ALA:HA	1:7:A:LEU:H	9	0.11
(1,463)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	3	0.11
(1,463)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	4	0.11
(1,463)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	6	0.11
(1,463)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	8	0.11
(1,463)	1:11:A:TRP:HH2	1:11:A:TRP:HZ3	9	0.11
(1,435)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	5	0.11
(1,392)	1:11:A:TRP:HH2	1:17:A:PRO:HA	2	0.11
(1,392)	1:11:A:TRP:HH2	1:17:A:PRO:HA	8	0.11
(1,391)	1:11:A:TRP:HH2	1:22:A:PRO:HA	7	0.11
(1,385)	1:11:A:TRP:HD1	1:23:A:PRO:HA	3	0.11
(1,385)	1:11:A:TRP:HD1	1:23:A:PRO:HA	4	0.11
(1,385)	1:11:A:TRP:HD1	1:23:A:PRO:HA	6	0.11
(1,385)	1:11:A:TRP:HD1	1:23:A:PRO:HA	7	0.11
(1,385)	1:11:A:TRP:HD1	1:23:A:PRO:HA	8	0.11
(1,376)	1:8:A:TYR:HA	1:11:A:TRP:HD1	1	0.11
(1,376)	1:8:A:TYR:HA	1:11:A:TRP:HD1	3	0.11
(1,376)	1:8:A:TYR:HA	1:11:A:TRP:HD1	6	0.11
(1,376)	1:8:A:TYR:HA	1:11:A:TRP:HD1	10	0.11
(1,362)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	3	0.11
(1,362)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	6	0.11
(1,360)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	7	0.11
(1,360)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	10	0.11
(1,347)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	10	0.11
(1,347)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	10	0.11
(1,347)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	10	0.11
(1,347)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	10	0.11
(1,347)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	10	0.11
(1,347)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	10	0.11
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	10	0.11
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	10	0.11
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	10	0.11
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	10	0.11
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	10	0.11
(1,327)	1:5:A:VAL:HA	1:8:A:TYR:HE1	4	0.11
(1,327)	1:5:A:VAL:HA	1:8:A:TYR:HE2	4	0.11
(1,233)	1:21:A:ARG:H	1:21:A:ARG:HD2	10	0.11
(1,208)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	1	0.11
(1,208)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	3	0.11
(1,208)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	4	0.11
(1,208)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	5	0.11
(1,208)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	8	0.11
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB2	1	0.11
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB2	4	0.11
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB2	8	0.11
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	2	0.11
(1,82)	1:7:A:LEU:H	1:7:A:LEU:HB3	4	0.11
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	6	0.1
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	6	0.1
(2,658)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	6	0.1
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	6	0.1
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	6	0.1
(2,658)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	6	0.1
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	6	0.1
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	6	0.1
(2,658)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	6	0.1
(2,656)	1:6:A:ARG:HG3	1:7:A:LEU:HD11	9	0.1
(2,656)	1:6:A:ARG:HG3	1:7:A:LEU:HD12	9	0.1
(2,656)	1:6:A:ARG:HG3	1:7:A:LEU:HD13	9	0.1
(2,653)	1:3:A:GLU:HB2	1:7:A:LEU:HD21	6	0.1
(2,653)	1:3:A:GLU:HB2	1:7:A:LEU:HD22	6	0.1
(2,653)	1:3:A:GLU:HB2	1:7:A:LEU:HD23	6	0.1
(2,648)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	9	0.1
(2,648)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	9	0.1
(2,648)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	9	0.1
(2,648)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	10	0.1
(2,648)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	10	0.1
(2,648)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	10	0.1
(2,619)	1:2:A:GLU:HB3	1:6:A:ARG:HG3	2	0.1
(2,619)	1:2:A:GLU:HB3	1:6:A:ARG:HG3	4	0.1
(2,618)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	10	0.1
(2,565)	1:2:A:GLU:HA	1:3:A:GLU:HB2	8	0.1
(2,565)	1:2:A:GLU:HA	1:3:A:GLU:HB2	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,506)	1:9:A:ILE:HG21	1:10:A:GLN:H	1	0.1
(2,506)	1:9:A:ILE:HG22	1:10:A:GLN:H	1	0.1
(2,506)	1:9:A:ILE:HG23	1:10:A:GLN:H	1	0.1
(2,506)	1:9:A:ILE:HG21	1:10:A:GLN:H	6	0.1
(2,506)	1:9:A:ILE:HG22	1:10:A:GLN:H	6	0.1
(2,506)	1:9:A:ILE:HG23	1:10:A:GLN:H	6	0.1
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD11	2	0.1
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD12	2	0.1
(2,505)	1:11:A:TRP:H	1:12:A:LEU:HD13	2	0.1
(2,455)	1:9:A:ILE:HG21	1:13:A:LYS:H	9	0.1
(2,455)	1:9:A:ILE:HG22	1:13:A:LYS:H	9	0.1
(2,455)	1:9:A:ILE:HG23	1:13:A:LYS:H	9	0.1
(2,344)	1:11:A:TRP:HD1	1:23:A:PRO:HA	10	0.1
(2,336)	1:8:A:TYR:HA	1:11:A:TRP:HD1	2	0.1
(2,336)	1:8:A:TYR:HA	1:11:A:TRP:HD1	4	0.1
(2,312)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	4	0.1
(2,312)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	4	0.1
(2,312)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	4	0.1
(2,312)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	4	0.1
(2,312)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	4	0.1
(2,312)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	4	0.1
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	4	0.1
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	4	0.1
(2,307)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	4	0.1
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	4	0.1
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	4	0.1
(2,307)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	4	0.1
(2,208)	1:21:A:ARG:H	1:21:A:ARG:HD2	3	0.1
(2,184)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	9	0.1
(2,179)	1:17:A:PRO:HA	1:17:A:PRO:HB2	5	0.1
(2,157)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	8	0.1
(2,157)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	8	0.1
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE1	1	0.1
(2,78)	1:8:A:TYR:HA	1:8:A:TYR:HE2	1	0.1
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	6	0.1
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	6	0.1
(1,736)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	6	0.1
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	6	0.1
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	6	0.1
(1,736)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	6	0.1
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	6	0.1
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	6	0.1
(1,734)	1:6:A:ARG:HG3	1:7:A:LEU:HD11	9	0.1
(1,734)	1:6:A:ARG:HG3	1:7:A:LEU:HD12	9	0.1
(1,734)	1:6:A:ARG:HG3	1:7:A:LEU:HD13	9	0.1
(1,730)	1:3:A:GLU:HB2	1:7:A:LEU:HD21	6	0.1
(1,730)	1:3:A:GLU:HB2	1:7:A:LEU:HD22	6	0.1
(1,730)	1:3:A:GLU:HB2	1:7:A:LEU:HD23	6	0.1
(1,724)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	9	0.1
(1,724)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	9	0.1
(1,724)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	9	0.1
(1,724)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	10	0.1
(1,724)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	10	0.1
(1,724)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	10	0.1
(1,693)	1:2:A:GLU:HB3	1:6:A:ARG:HG3	2	0.1
(1,693)	1:2:A:GLU:HB3	1:6:A:ARG:HG3	4	0.1
(1,692)	1:2:A:GLU:HB3	1:6:A:ARG:HG2	10	0.1
(1,637)	1:2:A:GLU:HA	1:3:A:GLU:HB2	8	0.1
(1,637)	1:2:A:GLU:HA	1:3:A:GLU:HB2	9	0.1
(1,575)	1:9:A:ILE:HG21	1:10:A:GLN:H	1	0.1
(1,575)	1:9:A:ILE:HG22	1:10:A:GLN:H	1	0.1
(1,575)	1:9:A:ILE:HG23	1:10:A:GLN:H	1	0.1
(1,575)	1:9:A:ILE:HG21	1:10:A:GLN:H	6	0.1
(1,575)	1:9:A:ILE:HG22	1:10:A:GLN:H	6	0.1
(1,575)	1:9:A:ILE:HG23	1:10:A:GLN:H	6	0.1
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD11	2	0.1
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD12	2	0.1
(1,574)	1:11:A:TRP:H	1:12:A:LEU:HD13	2	0.1
(1,516)	1:9:A:ILE:HG21	1:13:A:LYS:H	9	0.1
(1,516)	1:9:A:ILE:HG22	1:13:A:LYS:H	9	0.1
(1,516)	1:9:A:ILE:HG23	1:13:A:LYS:H	9	0.1
(1,385)	1:11:A:TRP:HD1	1:23:A:PRO:HA	10	0.1
(1,376)	1:8:A:TYR:HA	1:11:A:TRP:HD1	2	0.1
(1,376)	1:8:A:TYR:HA	1:11:A:TRP:HD1	4	0.1
(1,347)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	4	0.1
(1,347)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	4	0.1
(1,347)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	4	0.1
(1,347)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	4	0.1
(1,347)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	4	0.1
(1,347)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	4	0.1
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	4	0.1
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	4	0.1
(1,340)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	4	0.1
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	4	0.1
(1,340)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	4	0.1
(1,233)	1:21:A:ARG:H	1:21:A:ARG:HD2	3	0.1
(1,208)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	9	0.1
(1,203)	1:17:A:PRO:HA	1:17:A:PRO:HB2	5	0.1
(1,180)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	8	0.1
(1,180)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	8	0.1
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE1	1	0.1
(1,91)	1:8:A:TYR:HA	1:8:A:TYR:HE2	1	0.1

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found