



Full wwPDB NMR Structure Validation Report ⓘ

Mar 15, 2026 – 12:37 PM UTC

PDB ID : 9G2N / pdb_00009g2n
BMRB ID : 34933
Title : Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bDR) at 288K
Authors : Horvath, D.
Deposited on : 2024-07-11

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

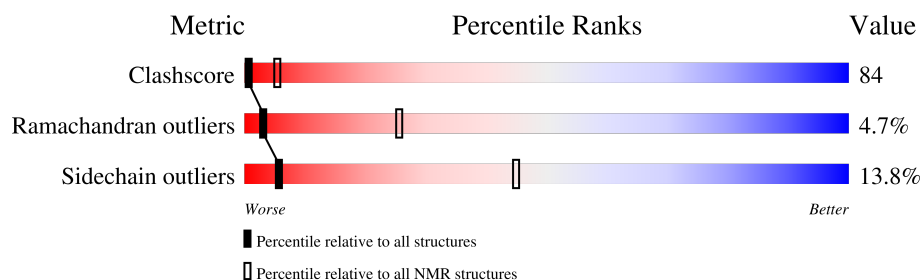
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	25	24% 40% 12% 24%

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:5-A:23 (19)	0.13	1

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. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 9, 10
2	7, 8

3 Entry composition

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.

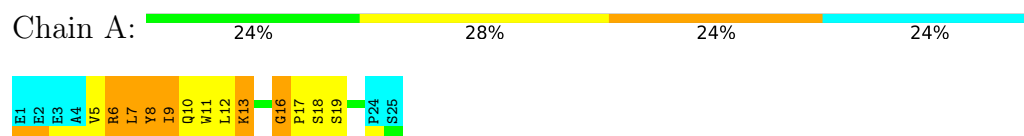
Mol	Chain	Residues	Atoms					Trace
1	A	25	Total	C	H	N	O	0
			385	123	189	34	39	

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

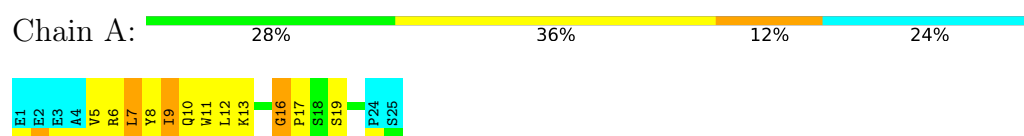
4.2.3 Score per residue for model 3

- Molecule 1: Exendin-4



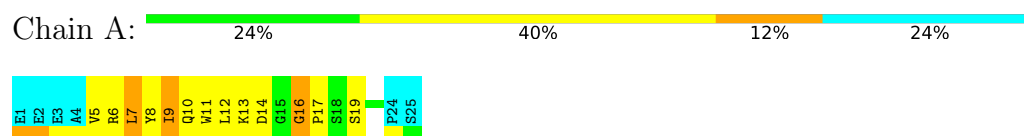
4.2.4 Score per residue for model 4

- Molecule 1: Exendin-4



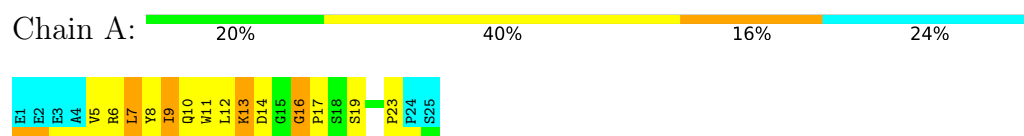
4.2.5 Score per residue for model 5

- Molecule 1: Exendin-4



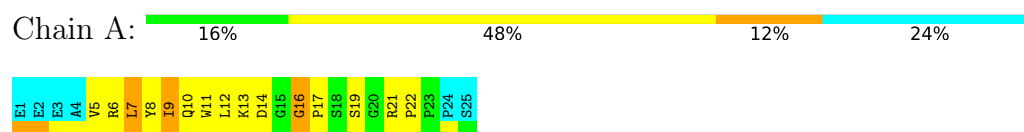
4.2.6 Score per residue for model 6

- Molecule 1: Exendin-4



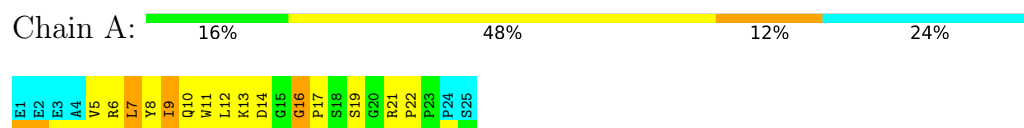
4.2.7 Score per residue for model 7

- Molecule 1: Exendin-4



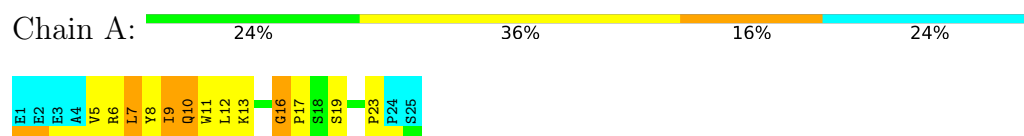
4.2.8 Score per residue for model 8

- Molecule 1: Exendin-4



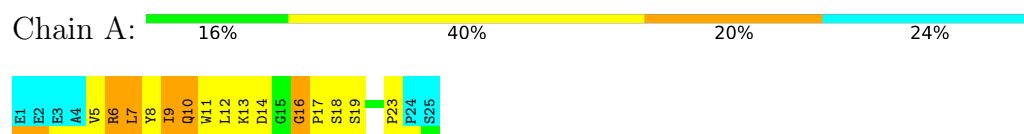
4.2.9 Score per residue for model 9

- Molecule 1: Exendin-4



4.2.10 Score per residue for model 10

- Molecule 1: Exendin-4



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	172
Number of shifts mapped to atoms	172
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

6.1 Standard geometry

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	1.41±0.04	1±0/156 (0.6± 0.0%)	1.48±0.04	1±1/214 (0.3± 0.4%)
All	All	1.41	10/1560 (0.6%)	1.48	6/2140 (0.3%)

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

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

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	9	ILE	N-CA	-6.74	1.38	1.46	10	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	PRO	CA-C-N	6.02	125.50	119.24	9	3
1	A	23	PRO	C-N-CA	6.02	125.50	119.24	9	3

There are no chirality outliers.

All unique planar outliers are listed below.

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

6.2 Too-close contacts ⓘ

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	150	152	152	25±3
All	All	1500	1520	1520	253

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 84.

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	0.86	1.46	8	10
1:A:6:ARG:O	1:A:10:GLN:HB2	0.75	1.81	9	10
1:A:9:ILE:O	1:A:13:LYS:HG2	0.73	1.84	10	10
1:A:8:TYR:O	1:A:11:TRP:HB3	0.71	1.85	8	10
1:A:7:LEU:HA	1:A:10:GLN:CB	0.69	2.17	2	10
1:A:7:LEU:HD12	1:A:8:TYR:N	0.69	2.02	7	10
1:A:7:LEU:HA	1:A:10:GLN:HB2	0.69	1.65	2	4
1:A:10:GLN:HA	1:A:13:LYS:HG2	0.67	1.65	10	10
1:A:7:LEU:HA	1:A:10:GLN:HB3	0.65	1.68	10	8
1:A:5:VAL:HG13	1:A:6:ARG:N	0.65	2.07	5	10
1:A:10:GLN:HA	1:A:13:LYS:CG	0.64	2.23	10	5
1:A:16:GLY:N	1:A:19:SER:HB3	0.63	2.09	10	9
1:A:5:VAL:O	1:A:9:ILE:HG13	0.60	1.96	6	10
1:A:9:ILE:CA	1:A:12:LEU:HD12	0.59	2.26	8	9
1:A:5:VAL:CG1	1:A:6:ARG:N	0.59	2.65	3	10
1:A:10:GLN:HA	1:A:10:GLN:NE2	0.57	2.15	8	8
1:A:8:TYR:O	1:A:12:LEU:HG	0.56	2.01	6	10
1:A:11:TRP:CH2	1:A:17:PRO:HD3	0.55	2.37	2	10
1:A:5:VAL:O	1:A:8:TYR:HB3	0.54	2.03	3	9
1:A:7:LEU:CA	1:A:10:GLN:HB2	0.53	2.32	2	2
1:A:21:ARG:HB3	1:A:22:PRO:CD	0.51	2.35	7	2
1:A:10:GLN:CA	1:A:13:LYS:HG2	0.50	2.36	10	5
1:A:7:LEU:CA	1:A:10:GLN:HB3	0.48	2.38	3	7
1:A:9:ILE:O	1:A:13:LYS:N	0.47	2.48	9	8
1:A:5:VAL:HA	1:A:8:TYR:HB3	0.47	1.85	9	6
1:A:8:TYR:CZ	1:A:12:LEU:HD11	0.46	2.44	3	9
1:A:7:LEU:C	1:A:10:GLN:HB3	0.46	2.36	8	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:TRP:O	1:A:14:ASP:HB2	0.46	2.10	1	5
1:A:11:TRP:CD2	1:A:16:GLY:HA2	0.45	2.47	5	8
1:A:21:ARG:HB3	1:A:22:PRO:HD2	0.45	1.88	8	2
1:A:12:LEU:HA	1:A:16:GLY:N	0.44	2.28	4	7
1:A:8:TYR:HE2	1:A:11:TRP:CZ3	0.43	2.31	3	1
1:A:8:TYR:CE1	1:A:12:LEU:HD11	0.43	2.47	3	1
1:A:5:VAL:C	1:A:8:TYR:HB3	0.43	2.39	6	2
1:A:9:ILE:O	1:A:12:LEU:HB2	0.43	2.14	10	4
1:A:10:GLN:HA	1:A:10:GLN:HE21	0.42	1.74	10	1
1:A:10:GLN:CA	1:A:10:GLN:HE21	0.42	2.27	10	1
1:A:5:VAL:CA	1:A:8:TYR:HB3	0.41	2.45	7	1
1:A:14:ASP:CB	1:A:19:SER:HB2	0.41	2.46	10	1
1:A:10:GLN:NE2	1:A:10:GLN:CA	0.40	2.79	9	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	19/25 (76%)	17±1 (88±4%)	1±1 (7±5%)	1±0 (5±2%)	3	25
All	All	190/250 (76%)	168 (88%)	13 (7%)	9 (5%)	3	25

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	16	GLY	9

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	16/21 (76%)	14±1 (86±7%)	2±1 (14±7%)	6	45
All	All	160/210 (76%)	138 (86%)	22 (14%)	6	45

All 6 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	7	LEU	10
1	A	13	LYS	4
1	A	10	GLN	3
1	A	6	ARG	2
1	A	18	SER	2
1	A	14	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

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 [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	172
Number of shifts mapped to atoms	172
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 [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 53%, i.e. 139 atoms were assigned a chemical shift out of a possible 264. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	38/92 (41%)	38/38 (100%)	0/38 (0%)	0/16 (0%)
Sidechain	91/151 (60%)	91/98 (93%)	0/45 (0%)	0/8 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	139/264 (53%)	139/146 (95%)	0/93 (0%)	0/25 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 171 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	114/188 (61%)	114/121 (94%)	0/59 (0%)	0/8 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	171/329 (52%)	171/180 (95%)	0/119 (0%)	0/30 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

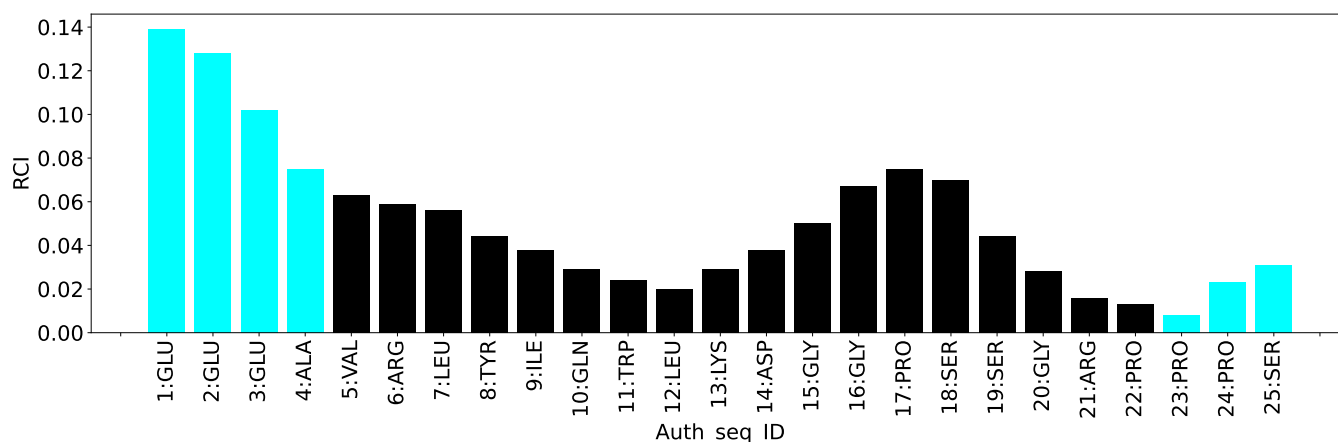
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	16	GLY	HA2	0.69	2.15 – 5.77	-9.0
1	A	23	PRO	HA	2.48	2.78 – 6.00	-5.9
1	A	23	PRO	HB2	0.30	0.37 – 3.78	-5.2

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	1380
Intra-residue ($ i-j =0$)	626
Sequential ($ i-j =1$)	298
Medium range ($ i-j >1$ and $ i-j <5$)	272
Long range ($ i-j \geq 5$)	184
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	55.2
Number of long range restraints per residue ¹	7.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	59.8	0.2
0.2-0.5 (Medium)	105.4	0.5
>0.5 (Large)	83.3	2.92

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

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

9 Distance violation analysis ⓘ

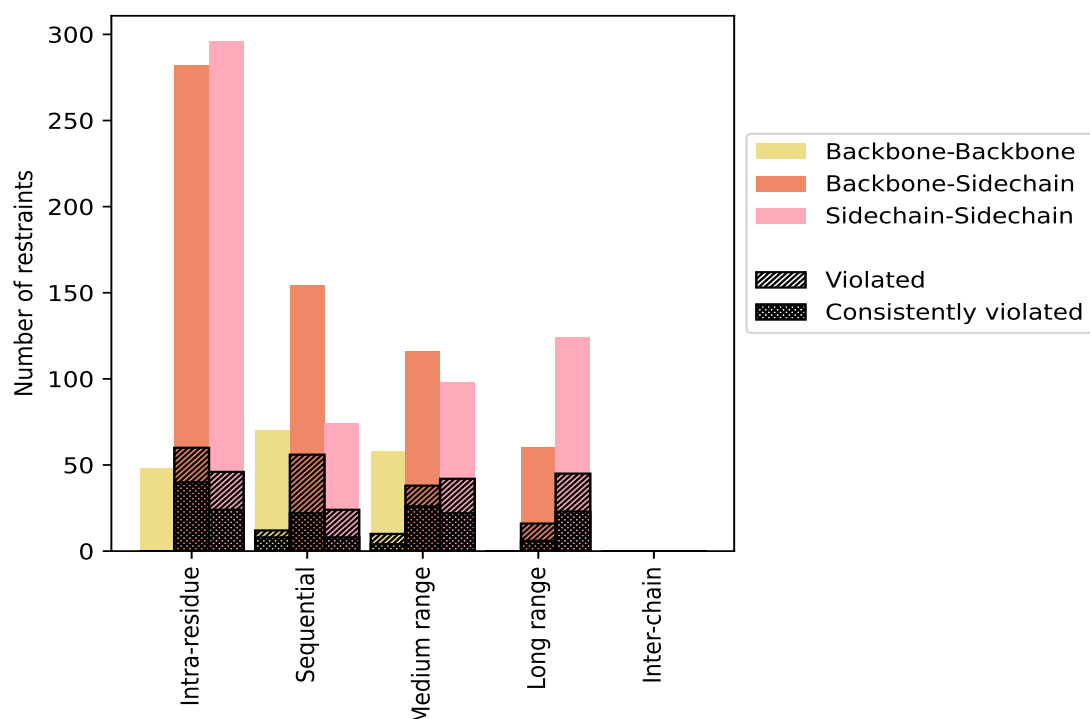
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	626	45.4	106	16.9	7.7	64	10.2	4.6
Backbone-Backbone	48	3.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	282	20.4	60	21.3	4.3	40	14.2	2.9
Sidechain-Sidechain	296	21.4	46	15.5	3.3	24	8.1	1.7
Sequential (i-j =1)	298	21.6	92	30.9	6.7	38	12.8	2.8
Backbone-Backbone	70	5.1	12	17.1	0.9	8	11.4	0.6
Backbone-Sidechain	154	11.2	56	36.4	4.1	22	14.3	1.6
Sidechain-Sidechain	74	5.4	24	32.4	1.7	8	10.8	0.6
Medium range (i-j >1 & i-j <5)	272	19.7	90	33.1	6.5	52	19.1	3.8
Backbone-Backbone	58	4.2	10	17.2	0.7	4	6.9	0.3
Backbone-Sidechain	116	8.4	38	32.8	2.8	26	22.4	1.9
Sidechain-Sidechain	98	7.1	42	42.9	3.0	22	22.4	1.6
Long range (i-j ≥5)	184	13.3	61	33.2	4.4	29	15.8	2.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	60	4.3	16	26.7	1.2	6	10.0	0.4
Sidechain-Sidechain	124	9.0	45	36.3	3.3	23	18.5	1.7
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	1380	100.0	349	25.3	25.3	183	13.3	13.3
Backbone-Backbone	176	12.8	22	12.5	1.6	12	6.8	0.9
Backbone-Sidechain	612	44.3	170	27.8	12.3	94	15.4	6.8
Sidechain-Sidechain	592	42.9	157	26.5	11.4	77	13.0	5.6

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

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



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

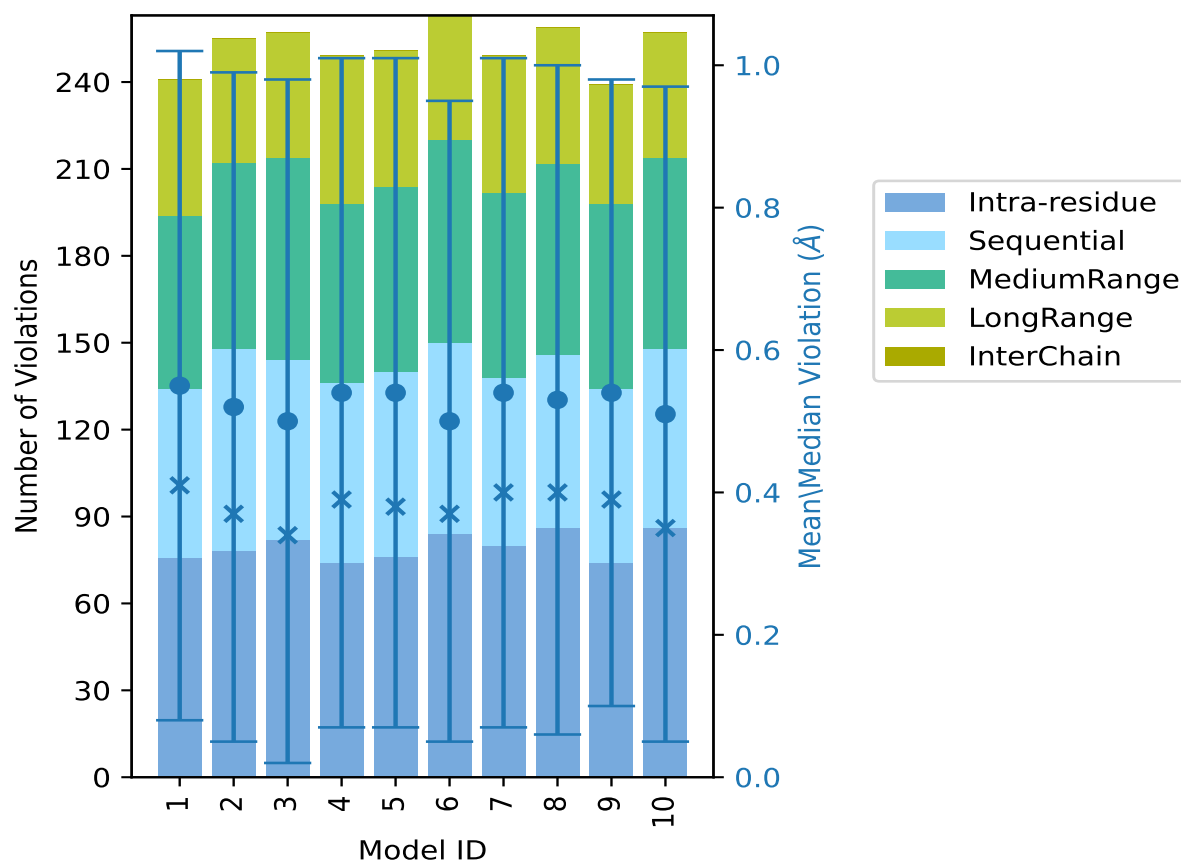
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	76	58	60	47	0	241	0.55	2.72	0.47	0.41
2	78	70	64	43	0	255	0.52	2.67	0.47	0.37
3	82	62	70	43	0	257	0.5	2.92	0.48	0.34
4	74	62	62	51	0	249	0.54	2.68	0.47	0.39
5	76	64	64	47	0	251	0.54	2.67	0.47	0.38
6	84	66	70	43	0	263	0.5	2.74	0.45	0.37
7	80	58	64	47	0	249	0.54	2.71	0.47	0.4
8	86	60	66	47	0	259	0.53	2.66	0.47	0.4
9	74	60	64	41	0	239	0.54	2.76	0.44	0.39
10	86	62	66	43	0	257	0.51	2.69	0.46	0.35

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

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1031(IR:520, SQ:206, MR:182, LR:123, 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	%
10	16	14	8	0	48	1	10.0
10	2	4	4	0	20	2	20.0
6	6	6	0	0	18	3	30.0

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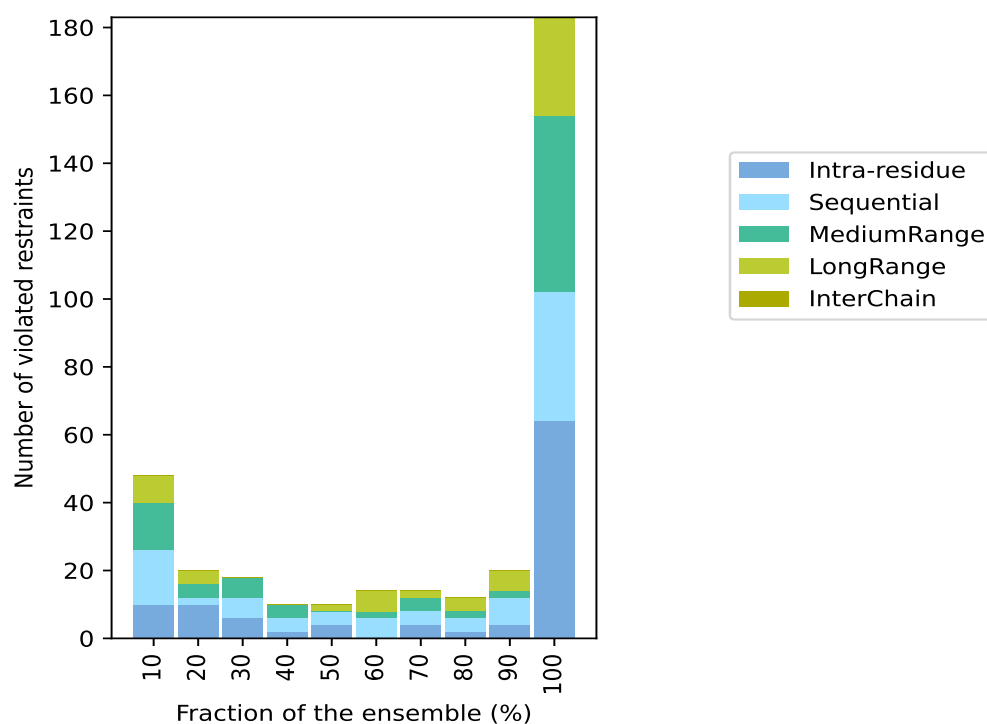
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	4	4	0	0	10	4	40.0
4	4	0	2	0	10	5	50.0
0	6	2	6	0	14	6	60.0
4	4	4	2	0	14	7	70.0
2	4	2	4	0	12	8	80.0
4	8	2	6	0	20	9	90.0
64	38	52	29	0	183	10	100.0

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

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

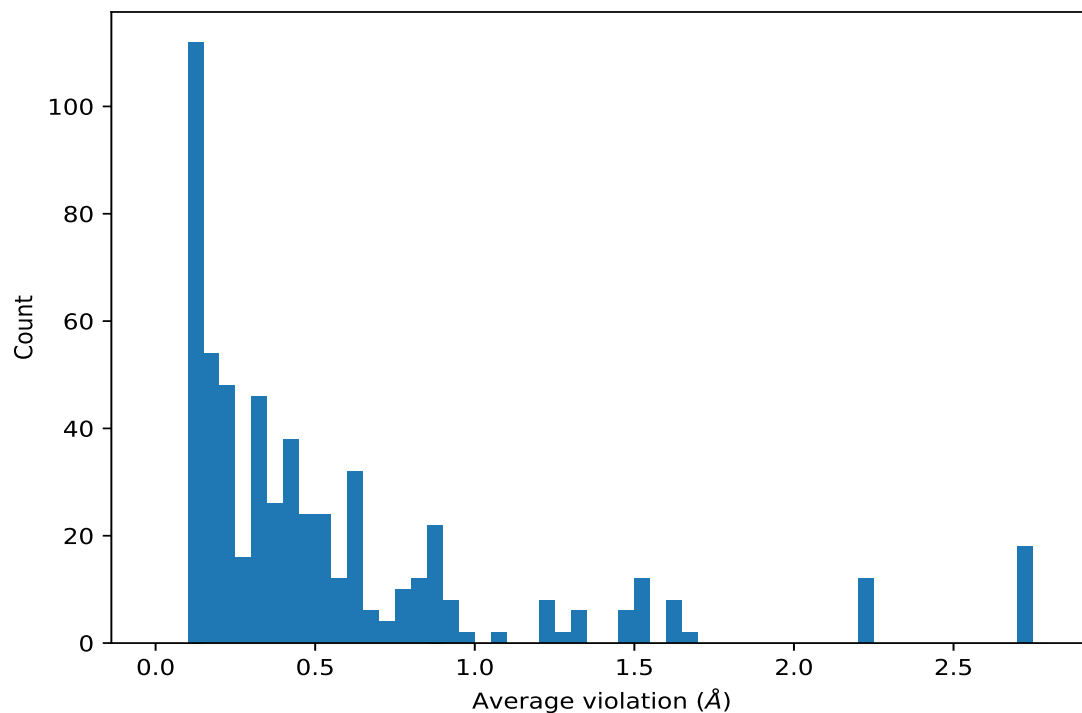


9.4 Most violated distance restraints in the ensemble ⓘ

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 [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	10	2.72	0.07	2.7
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	10	2.72	0.07	2.7
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	10	2.72	0.07	2.7
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	10	2.72	0.07	2.7
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	10	2.72	0.07	2.7
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	10	2.72	0.07	2.7
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	10	2.72	0.07	2.7
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	10	2.72	0.07	2.7
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	10	2.72	0.07	2.7
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	10	2.72	0.07	2.7
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	10	2.72	0.07	2.7
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	10	2.72	0.07	2.7
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	10	2.72	0.07	2.7
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	10	2.72	0.07	2.7
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	10	2.72	0.07	2.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	10	2.72	0.07	2.7
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	10	2.72	0.07	2.7
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	10	2.72	0.07	2.7
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	10	2.24	0.14	2.22
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	10	2.24	0.14	2.22
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	10	2.24	0.14	2.22
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	10	2.24	0.14	2.22
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	10	2.24	0.14	2.22
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	10	2.24	0.14	2.22
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	10	2.24	0.14	2.22
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	10	2.24	0.14	2.22
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	10	2.24	0.14	2.22
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	10	2.24	0.14	2.22
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	10	2.24	0.14	2.22
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	10	2.24	0.14	2.22
(1,527)	1:2:A:GLU:HA	1:5:A:VAL:HB	10	1.67	0.05	1.68
(4,51)	1:2:A:GLU:HA	1:5:A:VAL:HB	10	1.67	0.05	1.68
(1,688)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	10	1.64	0.13	1.65
(1,688)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	10	1.64	0.13	1.65
(1,688)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	10	1.64	0.13	1.65
(4,74)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	10	1.64	0.13	1.65
(4,74)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	10	1.64	0.13	1.65
(4,74)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	10	1.64	0.13	1.65
(1,674)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	10	1.61	0.35	1.77
(3,603)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	10	1.61	0.35	1.77
(1,648)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	10	1.53	0.35	1.68
(1,648)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	10	1.53	0.35	1.68
(1,648)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	10	1.53	0.35	1.68
(4,64)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	10	1.53	0.35	1.68
(4,64)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	10	1.53	0.35	1.68
(4,64)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	10	1.53	0.35	1.68
(1,651)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	10	1.52	0.11	1.56
(1,651)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	10	1.52	0.11	1.56
(1,651)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	10	1.52	0.11	1.56
(4,65)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	10	1.52	0.11	1.56
(4,65)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	10	1.52	0.11	1.56
(4,65)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	10	1.52	0.11	1.56
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	1.46	0.01	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	1.46	0.01	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	1.46	0.01	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	1.46	0.01	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	1.46	0.01	1.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	1.46	0.01	1.46
(1,357)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	1.33	0.04	1.34
(3,326)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	1.33	0.04	1.34
(1,406)	1:10:A:GLN:H	1:13:A:LYS:H	10	1.32	0.03	1.32
(4,37)	1:10:A:GLN:H	1:13:A:LYS:H	10	1.32	0.03	1.32
(1,672)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	10	1.3	0.25	1.45
(3,601)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	10	1.3	0.25	1.45
(1,566)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	10	1.27	0.25	1.11
(3,510)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	10	1.27	0.25	1.11
(1,356)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	10	1.23	0.15	1.27
(3,325)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	10	1.23	0.15	1.27
(1,598)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	10	1.23	0.11	1.2
(1,598)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	10	1.23	0.11	1.2
(1,598)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	10	1.23	0.11	1.2
(4,59)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	10	1.23	0.11	1.2
(4,59)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	10	1.23	0.11	1.2
(4,59)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	10	1.23	0.11	1.2
(1,380)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.05	0.03	1.04
(4,32)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.05	0.03	1.04
(1,396)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	10	0.96	0.0	0.96
(4,35)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	10	0.96	0.0	0.96
(1,689)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	10	0.92	0.06	0.92
(1,689)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	10	0.92	0.06	0.92
(1,689)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	10	0.92	0.06	0.92
(3,614)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	10	0.92	0.06	0.92
(3,614)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	10	0.92	0.06	0.92
(3,614)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	10	0.92	0.06	0.92
(1,353)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	10	0.89	0.03	0.9
(3,322)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	10	0.89	0.03	0.9
(1,681)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	10	0.88	0.2	0.94
(1,681)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	10	0.88	0.2	0.94
(1,681)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	10	0.88	0.2	0.94
(4,72)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	10	0.88	0.2	0.94
(4,72)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	10	0.88	0.2	0.94
(4,72)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	10	0.88	0.2	0.94
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	0.86	0.07	0.9
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	0.86	0.07	0.9
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	0.86	0.07	0.9
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	0.86	0.07	0.9
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	0.86	0.07	0.9
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	0.86	0.07	0.9
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.86	0.02	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.86	0.02	0.86
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.86	0.02	0.86
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.86	0.02	0.86
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.86	0.02	0.86
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.86	0.02	0.86
(1,523)	1:11:A:TRP:HA	1:14:A:ASP:HB3	10	0.85	0.02	0.85
(3,473)	1:11:A:TRP:HA	1:14:A:ASP:HB3	10	0.85	0.02	0.85
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	10	0.83	0.39	0.97
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	10	0.83	0.39	0.97
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	10	0.83	0.39	0.97
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	10	0.83	0.39	0.97
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	10	0.83	0.39	0.97
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	10	0.83	0.39	0.97
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	10	0.83	0.39	0.97
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	10	0.83	0.39	0.97
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	10	0.83	0.39	0.97
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	10	0.83	0.39	0.97
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	10	0.83	0.39	0.97
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	10	0.83	0.39	0.97
(1,469)	1:7:A:LEU:HD11	1:10:A:GLN:H	10	0.79	0.06	0.8
(1,469)	1:7:A:LEU:HD12	1:10:A:GLN:H	10	0.79	0.06	0.8
(1,469)	1:7:A:LEU:HD13	1:10:A:GLN:H	10	0.79	0.06	0.8
(4,46)	1:7:A:LEU:HD11	1:10:A:GLN:H	10	0.79	0.06	0.8
(4,46)	1:7:A:LEU:HD12	1:10:A:GLN:H	10	0.79	0.06	0.8
(4,46)	1:7:A:LEU:HD13	1:10:A:GLN:H	10	0.79	0.06	0.8
(1,483)	1:5:A:VAL:HB	1:6:A:ARG:H	10	0.79	0.08	0.83
(4,48)	1:5:A:VAL:HB	1:6:A:ARG:H	10	0.79	0.08	0.83
(1,623)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.78	0.09	0.77
(3,560)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.78	0.09	0.77
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.74	0.02	0.74
(4,16)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.74	0.02	0.74
(1,638)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.73	0.2	0.79
(3,575)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.73	0.2	0.79
(1,424)	1:1:A:GLU:HG2	1:4:A:ALA:H	10	0.67	0.51	0.37
(1,424)	1:1:A:GLU:HG3	1:4:A:ALA:H	10	0.67	0.51	0.37
(4,39)	1:1:A:GLU:HG2	1:4:A:ALA:H	10	0.67	0.51	0.37
(4,39)	1:1:A:GLU:HG3	1:4:A:ALA:H	10	0.67	0.51	0.37
(1,168)	1:14:A:ASP:H	1:14:A:ASP:HB3	10	0.63	0.07	0.65
(3,146)	1:14:A:ASP:H	1:14:A:ASP:HB3	10	0.63	0.07	0.65
(1,540)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.61	0.04	0.6
(3,487)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.61	0.04	0.6
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.6	0.22	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.6	0.22	0.46
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.6	0.22	0.46
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.6	0.22	0.46
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.6	0.22	0.46
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.6	0.22	0.46
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.6	0.22	0.46
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.6	0.22	0.46
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.6	0.22	0.46
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.6	0.22	0.46
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.6	0.22	0.46
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.6	0.22	0.46
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.6	0.22	0.46
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.6	0.22	0.46
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.6	0.22	0.46
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.6	0.22	0.46
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.6	0.22	0.46
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.6	0.22	0.46
(1,228)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.59	0.01	0.6
(3,205)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.59	0.01	0.6
(1,459)	1:8:A:TYR:H	1:24:A:PRO:HB3	10	0.58	0.35	0.74
(3,417)	1:8:A:TYR:H	1:24:A:PRO:HB3	10	0.58	0.35	0.74
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD21	10	0.55	0.1	0.51
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD22	10	0.55	0.1	0.51
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD23	10	0.55	0.1	0.51
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD21	10	0.55	0.1	0.51
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD22	10	0.55	0.1	0.51
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD23	10	0.55	0.1	0.51
(1,559)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	10	0.55	0.13	0.51
(4,55)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	10	0.55	0.13	0.51
(1,352)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	10	0.54	0.06	0.56
(3,321)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	10	0.54	0.06	0.56
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD11	10	0.53	0.06	0.52
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD12	10	0.53	0.06	0.52
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD13	10	0.53	0.06	0.52
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	10	0.53	0.06	0.52
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	10	0.53	0.06	0.52
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	10	0.53	0.06	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.52	0.01	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.52	0.01	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.52	0.01	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.52	0.01	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.52	0.01	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.52	0.01	0.52
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	10	0.52	0.12	0.56
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	10	0.52	0.12	0.56
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	10	0.52	0.12	0.56
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	10	0.52	0.12	0.56
(1,285)	1:24:A:PRO:HA	1:25:A:SER:H	10	0.51	0.19	0.4
(4,25)	1:24:A:PRO:HA	1:25:A:SER:H	10	0.51	0.19	0.4
(1,534)	1:3:A:GLU:HA	1:6:A:ARG:HB2	10	0.51	0.4	0.29
(4,53)	1:3:A:GLU:HA	1:6:A:ARG:HB2	10	0.51	0.4	0.29
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.48	0.02	0.48
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.48	0.02	0.48
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.48	0.02	0.48
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.48	0.02	0.48
(1,49)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.48	0.14	0.5
(4,7)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.48	0.14	0.5
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	10	0.48	0.14	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	10	0.48	0.14	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	10	0.48	0.14	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	10	0.48	0.14	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	10	0.48	0.14	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	10	0.48	0.14	0.44
(1,440)	1:12:A:LEU:HA	1:13:A:LYS:H	10	0.47	0.02	0.47
(4,41)	1:12:A:LEU:HA	1:13:A:LYS:H	10	0.47	0.02	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.46	0.01	0.46
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.46	0.01	0.46
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.46	0.01	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.46	0.01	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.46	0.01	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.46	0.01	0.46
(1,397)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.44	0.01	0.44
(4,36)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.44	0.01	0.44
(1,125)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.43	0.06	0.44
(4,21)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.43	0.06	0.44
(1,119)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	10	0.43	0.03	0.44
(3,100)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	10	0.43	0.03	0.44
(1,460)	1:7:A:LEU:HB2	1:8:A:TYR:H	10	0.42	0.05	0.44
(4,43)	1:7:A:LEU:HB2	1:8:A:TYR:H	10	0.42	0.05	0.44
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.42	0.0	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.42	0.0	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.42	0.0	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.42	0.0	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.42	0.0	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.42	0.0	0.42
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG11	10	0.41	0.01	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG12	10	0.41	0.01	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG13	10	0.41	0.01	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG11	10	0.41	0.01	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG12	10	0.41	0.01	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG13	10	0.41	0.01	0.4
(1,656)	1:8:A:TYR:HA	1:9:A:ILE:H	10	0.4	0.01	0.4
(2,1)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	10	0.4	0.15	0.4
(2,1)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	10	0.4	0.15	0.4
(4,67)	1:8:A:TYR:HA	1:9:A:ILE:H	10	0.4	0.01	0.4
(1,381)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.4	0.02	0.39
(4,33)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.4	0.02	0.39
(1,445)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.38	0.01	0.38
(4,42)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.38	0.01	0.38
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.37	0.1	0.42
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.37	0.1	0.42
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.37	0.1	0.42
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.37	0.1	0.42
(1,422)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.36	0.03	0.36
(3,384)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.36	0.03	0.36
(1,653)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	10	0.36	0.12	0.31
(1,653)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	10	0.36	0.12	0.31
(1,653)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	10	0.36	0.12	0.31
(4,66)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	10	0.36	0.12	0.31
(4,66)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	10	0.36	0.12	0.31
(4,66)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	10	0.36	0.12	0.31
(1,346)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.36	0.03	0.36
(4,30)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.36	0.03	0.36
(1,665)	1:7:A:LEU:HA	1:8:A:TYR:H	10	0.33	0.01	0.32
(4,68)	1:7:A:LEU:HA	1:8:A:TYR:H	10	0.33	0.01	0.32
(1,124)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.33	0.04	0.34
(4,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.33	0.04	0.34
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.32	0.02	0.32
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.32	0.02	0.32
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.32	0.01	0.32
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.32	0.01	0.32
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD21	10	0.31	0.03	0.32
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD22	10	0.31	0.03	0.32
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD23	10	0.31	0.03	0.32
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD21	10	0.31	0.03	0.32
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD22	10	0.31	0.03	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD23	10	0.31	0.03	0.32
(1,585)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	10	0.31	0.09	0.36
(1,585)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	10	0.31	0.09	0.36
(1,585)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	10	0.31	0.09	0.36
(3,528)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	10	0.31	0.09	0.36
(3,528)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	10	0.31	0.09	0.36
(3,528)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	10	0.31	0.09	0.36
(1,613)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	0.3	0.06	0.32
(1,613)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	0.3	0.06	0.32
(1,613)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	0.3	0.06	0.32
(4,62)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	0.3	0.06	0.32
(4,62)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	0.3	0.06	0.32
(4,62)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	0.3	0.06	0.32
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD2	10	0.3	0.07	0.3
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD3	10	0.3	0.07	0.3
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD2	10	0.3	0.07	0.3
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD3	10	0.3	0.07	0.3
(1,315)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.29	0.03	0.3
(3,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.29	0.03	0.3
(1,35)	1:6:A:ARG:HA	1:6:A:ARG:HG2	10	0.28	0.15	0.24
(4,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	10	0.28	0.15	0.24
(1,529)	1:1:A:GLU:HB2	1:2:A:GLU:HA	10	0.26	0.1	0.32
(4,52)	1:1:A:GLU:HB2	1:2:A:GLU:HA	10	0.26	0.1	0.32
(1,439)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.25	0.02	0.24
(4,40)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.25	0.02	0.24
(1,417)	1:3:A:GLU:H	1:5:A:VAL:HB	10	0.25	0.06	0.24
(4,38)	1:3:A:GLU:H	1:5:A:VAL:HB	10	0.25	0.06	0.24
(1,494)	1:7:A:LEU:HA	1:11:A:TRP:H	10	0.24	0.02	0.24
(4,50)	1:7:A:LEU:HA	1:11:A:TRP:H	10	0.24	0.02	0.24
(1,532)	1:8:A:TYR:HA	1:24:A:PRO:HB3	10	0.24	0.06	0.22
(3,480)	1:8:A:TYR:HA	1:24:A:PRO:HB3	10	0.24	0.06	0.22
(1,60)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.24	0.0	0.24
(4,9)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.24	0.0	0.24
(1,68)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.24	0.05	0.24
(4,10)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.24	0.05	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.23	0.04	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.23	0.04	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.23	0.04	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.23	0.04	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.23	0.04	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.23	0.04	0.24
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.23	0.06	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.23	0.06	0.22
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.23	0.06	0.22
(3,423)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.23	0.06	0.22
(3,423)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.23	0.06	0.22
(3,423)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.23	0.06	0.22
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	10	0.22	0.04	0.22
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	10	0.22	0.04	0.22
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	10	0.22	0.04	0.22
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	10	0.22	0.04	0.22
(1,205)	1:19:A:SER:HA	1:19:A:SER:HB3	10	0.21	0.02	0.22
(4,23)	1:19:A:SER:HA	1:19:A:SER:HB3	10	0.21	0.02	0.21
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE1	10	0.2	0.03	0.21
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE2	10	0.2	0.03	0.21
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE1	10	0.2	0.03	0.21
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE2	10	0.2	0.03	0.21
(1,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.2	0.02	0.2
(3,224)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.2	0.02	0.2
(1,449)	1:12:A:LEU:HD11	1:16:A:GLY:H	10	0.19	0.02	0.2
(1,449)	1:12:A:LEU:HD12	1:16:A:GLY:H	10	0.19	0.02	0.2
(1,449)	1:12:A:LEU:HD13	1:16:A:GLY:H	10	0.19	0.02	0.2
(3,407)	1:12:A:LEU:HD11	1:16:A:GLY:H	10	0.19	0.02	0.2
(3,407)	1:12:A:LEU:HD12	1:16:A:GLY:H	10	0.19	0.02	0.2
(3,407)	1:12:A:LEU:HD13	1:16:A:GLY:H	10	0.19	0.02	0.2
(1,476)	1:11:A:TRP:H	1:24:A:PRO:HG2	10	0.19	0.1	0.16
(3,429)	1:11:A:TRP:H	1:24:A:PRO:HG2	10	0.19	0.1	0.16
(1,391)	1:8:A:TYR:HD1	1:11:A:TRP:H	10	0.18	0.03	0.18
(1,391)	1:8:A:TYR:HD2	1:11:A:TRP:H	10	0.18	0.03	0.18
(3,357)	1:8:A:TYR:HD1	1:11:A:TRP:H	10	0.18	0.03	0.18
(3,357)	1:8:A:TYR:HD2	1:11:A:TRP:H	10	0.18	0.03	0.18
(1,389)	1:8:A:TYR:HD1	1:12:A:LEU:H	10	0.18	0.04	0.18
(1,389)	1:8:A:TYR:HD2	1:12:A:LEU:H	10	0.18	0.04	0.18
(4,34)	1:8:A:TYR:HD1	1:12:A:LEU:H	10	0.18	0.04	0.18
(4,34)	1:8:A:TYR:HD2	1:12:A:LEU:H	10	0.18	0.04	0.18
(1,186)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	10	0.15	0.01	0.15
(3,164)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	10	0.15	0.01	0.15
(1,488)	1:10:A:GLN:H	1:11:A:TRP:HB2	10	0.14	0.02	0.14
(3,439)	1:10:A:GLN:H	1:11:A:TRP:HB2	10	0.14	0.02	0.13
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG21	10	0.13	0.02	0.13
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG22	10	0.13	0.02	0.13
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG23	10	0.13	0.02	0.13
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG21	10	0.13	0.02	0.13
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG22	10	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG23	10	0.13	0.02	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD21	10	0.13	0.01	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD22	10	0.13	0.01	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD23	10	0.13	0.01	0.13
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.13	0.01	0.13
(3,177)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.13	0.01	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD21	10	0.13	0.01	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD22	10	0.13	0.01	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD23	10	0.13	0.01	0.13
(1,310)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	0.62	0.03	0.62
(1,310)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	0.62	0.03	0.62
(3,282)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	0.62	0.03	0.62
(3,282)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	0.62	0.03	0.62
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	9	0.47	0.13	0.52
(3,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	9	0.47	0.13	0.52
(1,374)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	9	0.39	0.02	0.4
(3,343)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	9	0.39	0.02	0.4
(1,350)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	9	0.38	0.01	0.38
(3,319)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	9	0.38	0.01	0.38
(1,553)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	9	0.27	0.08	0.26
(3,499)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	9	0.27	0.08	0.26
(1,669)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	9	0.18	0.04	0.17
(1,669)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	9	0.18	0.04	0.17
(4,69)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	9	0.18	0.04	0.17
(4,69)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	9	0.18	0.04	0.17
(1,545)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	9	0.18	0.05	0.17
(3,491)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	9	0.18	0.05	0.17
(1,149)	1:13:A:LYS:HA	1:13:A:LYS:HG3	9	0.17	0.06	0.15
(3,128)	1:13:A:LYS:HA	1:13:A:LYS:HG3	9	0.17	0.06	0.15
(1,486)	1:10:A:GLN:HG2	1:11:A:TRP:H	9	0.17	0.04	0.17
(3,437)	1:10:A:GLN:HG2	1:11:A:TRP:H	9	0.17	0.04	0.17
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	9	0.15	0.04	0.16
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	9	0.15	0.04	0.16
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	9	0.15	0.04	0.16
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	9	0.15	0.04	0.16
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	9	0.15	0.04	0.16
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	9	0.15	0.04	0.16
(1,332)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	8	0.44	0.02	0.44
(3,303)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	8	0.44	0.02	0.44
(1,136)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	8	0.36	0.01	0.36
(3,115)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	8	0.36	0.01	0.36
(1,538)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	8	0.32	0.08	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,538)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	8	0.32	0.08	0.36
(3,485)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	8	0.32	0.08	0.36
(3,485)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	8	0.32	0.08	0.36
(1,631)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	8	0.3	0.07	0.32
(3,568)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	8	0.3	0.07	0.32
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	8	0.14	0.03	0.13
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	8	0.14	0.03	0.13
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	8	0.14	0.03	0.13
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	8	0.14	0.03	0.13
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	8	0.14	0.03	0.13
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	8	0.14	0.03	0.13
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	8	0.14	0.03	0.13
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	8	0.14	0.03	0.13
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	8	0.14	0.03	0.13
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	8	0.14	0.02	0.13
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	8	0.14	0.02	0.13
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	8	0.14	0.02	0.13
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	8	0.14	0.02	0.13
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	8	0.14	0.02	0.13
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	8	0.14	0.02	0.13
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	8	0.14	0.02	0.13
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	8	0.14	0.02	0.13
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	8	0.14	0.02	0.13
(1,317)	1:8:A:TYR:HD1	1:9:A:ILE:HB	8	0.12	0.02	0.12
(1,317)	1:8:A:TYR:HD2	1:9:A:ILE:HB	8	0.12	0.02	0.12
(3,289)	1:8:A:TYR:HD1	1:9:A:ILE:HB	8	0.12	0.02	0.12
(3,289)	1:8:A:TYR:HD2	1:9:A:ILE:HB	8	0.12	0.02	0.12
(1,418)	1:2:A:GLU:HG2	1:3:A:GLU:H	7	0.91	0.05	0.91
(3,380)	1:2:A:GLU:HG2	1:3:A:GLU:H	7	0.91	0.05	0.91
(1,1)	1:2:A:GLU:HA	1:3:A:GLU:H	7	0.37	0.03	0.38
(4,1)	1:2:A:GLU:HA	1:3:A:GLU:H	7	0.37	0.03	0.38
(1,14)	1:3:A:GLU:H	1:3:A:GLU:HB3	7	0.34	0.05	0.35
(4,3)	1:3:A:GLU:H	1:3:A:GLU:HB3	7	0.34	0.05	0.35
(1,675)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	7	0.22	0.02	0.22
(1,675)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	7	0.22	0.02	0.22
(1,675)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	7	0.22	0.02	0.22
(4,71)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	7	0.22	0.02	0.22
(4,71)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	7	0.22	0.02	0.22
(4,71)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	7	0.22	0.02	0.22
(1,322)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	7	0.21	0.07	0.24
(1,322)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	7	0.21	0.07	0.24
(3,293)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	7	0.21	0.07	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,293)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	7	0.21	0.07	0.24
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	7	0.15	0.02	0.16
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	7	0.15	0.02	0.16
(1,646)	1:2:A:GLU:HG3	1:5:A:VAL:HB	7	0.15	0.01	0.15
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	7	0.15	0.02	0.15
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	7	0.15	0.02	0.15
(3,583)	1:2:A:GLU:HG3	1:5:A:VAL:HB	7	0.15	0.01	0.15
(1,679)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	6	0.6	0.04	0.6
(1,679)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	6	0.6	0.04	0.6
(1,679)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	6	0.6	0.04	0.6
(3,607)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	6	0.6	0.04	0.6
(3,607)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	6	0.6	0.04	0.6
(3,607)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	6	0.6	0.04	0.6
(1,510)	1:24:A:PRO:HB3	1:25:A:SER:H	6	0.47	0.02	0.47
(3,460)	1:24:A:PRO:HB3	1:25:A:SER:H	6	0.47	0.02	0.47
(1,678)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	6	0.41	0.05	0.43
(1,678)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	6	0.41	0.05	0.43
(1,678)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	6	0.41	0.05	0.43
(3,606)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	6	0.41	0.05	0.43
(3,606)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	6	0.41	0.05	0.43
(3,606)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	6	0.41	0.05	0.43
(1,673)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	6	0.24	0.04	0.24
(3,602)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	6	0.24	0.04	0.24
(1,463)	1:7:A:LEU:HD11	1:8:A:TYR:H	6	0.13	0.03	0.12
(1,463)	1:7:A:LEU:HD12	1:8:A:TYR:H	6	0.13	0.03	0.12
(1,463)	1:7:A:LEU:HD13	1:8:A:TYR:H	6	0.13	0.03	0.12
(4,44)	1:7:A:LEU:HD11	1:8:A:TYR:H	6	0.13	0.03	0.12
(4,44)	1:7:A:LEU:HD12	1:8:A:TYR:H	6	0.13	0.03	0.12
(4,44)	1:7:A:LEU:HD13	1:8:A:TYR:H	6	0.13	0.03	0.12
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	6	0.13	0.02	0.12
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	6	0.13	0.02	0.12
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	6	0.13	0.02	0.12
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	6	0.13	0.02	0.12
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	6	0.13	0.02	0.12
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	6	0.13	0.02	0.12
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	6	0.13	0.02	0.12
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	6	0.13	0.02	0.12
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	6	0.13	0.02	0.12
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	6	0.13	0.02	0.12
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	6	0.13	0.02	0.12
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	6	0.13	0.02	0.12
(1,461)	1:8:A:TYR:H	1:9:A:ILE:HG13	6	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,418)	1:8:A:TYR:H	1:9:A:ILE:HG13	6	0.12	0.01	0.11
(1,248)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.5	0.18	0.64
(4,24)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.5	0.18	0.64
(1,624)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	5	0.19	0.04	0.18
(3,561)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	5	0.19	0.04	0.18
(1,234)	1:21:A:ARG:HA	1:22:A:PRO:HD2	5	0.18	0.06	0.16
(3,211)	1:21:A:ARG:HA	1:22:A:PRO:HD2	5	0.18	0.06	0.16
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	5	0.13	0.01	0.14
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	5	0.13	0.01	0.14
(1,153)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	5	0.13	0.01	0.14
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	5	0.13	0.01	0.14
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	5	0.13	0.01	0.14
(3,132)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	5	0.13	0.01	0.14
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD11	5	0.11	0.0	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD12	5	0.11	0.0	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD13	5	0.11	0.0	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD11	5	0.11	0.0	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD12	5	0.11	0.0	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD13	5	0.11	0.0	0.11
(1,508)	1:23:A:PRO:HB3	1:25:A:SER:H	4	0.42	0.1	0.45
(3,458)	1:23:A:PRO:HB3	1:25:A:SER:H	4	0.42	0.1	0.45
(1,431)	1:9:A:ILE:H	1:10:A:GLN:HB3	4	0.32	0.21	0.3
(3,392)	1:9:A:ILE:H	1:10:A:GLN:HB3	4	0.32	0.21	0.3
(1,617)	1:2:A:GLU:HB2	1:4:A:ALA:H	4	0.26	0.09	0.3
(1,617)	1:2:A:GLU:HB3	1:4:A:ALA:H	4	0.26	0.09	0.3
(3,555)	1:2:A:GLU:HB2	1:4:A:ALA:H	4	0.26	0.09	0.3
(3,555)	1:2:A:GLU:HB3	1:4:A:ALA:H	4	0.26	0.09	0.3
(1,159)	1:13:A:LYS:H	1:13:A:LYS:HD2	4	0.13	0.02	0.13
(3,138)	1:13:A:LYS:H	1:13:A:LYS:HD2	4	0.13	0.02	0.13
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	4	0.12	0.01	0.12
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	4	0.12	0.01	0.12
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	4	0.12	0.01	0.12
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	4	0.12	0.01	0.12
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	4	0.12	0.01	0.12
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	4	0.12	0.01	0.12
(1,454)	1:18:A:SER:HB2	1:19:A:SER:H	3	0.37	0.17	0.49
(3,412)	1:18:A:SER:HB2	1:19:A:SER:H	3	0.37	0.17	0.49
(1,375)	1:21:A:ARG:HD3	1:21:A:ARG:HH11	3	0.22	0.06	0.26
(1,375)	1:21:A:ARG:HD3	1:21:A:ARG:HH12	3	0.22	0.06	0.26
(3,344)	1:21:A:ARG:HD3	1:21:A:ARG:HH11	3	0.22	0.06	0.26
(3,344)	1:21:A:ARG:HD3	1:21:A:ARG:HH12	3	0.22	0.06	0.26
(1,658)	1:2:A:GLU:HG3	1:4:A:ALA:H	3	0.19	0.01	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,591)	1:2:A:GLU:HG3	1:4:A:ALA:H	3	0.19	0.01	0.19
(1,649)	1:5:A:VAL:HG11	1:6:A:ARG:HG3	3	0.15	0.03	0.14
(1,649)	1:5:A:VAL:HG12	1:6:A:ARG:HG3	3	0.15	0.03	0.14
(1,649)	1:5:A:VAL:HG13	1:6:A:ARG:HG3	3	0.15	0.03	0.14
(3,585)	1:5:A:VAL:HG11	1:6:A:ARG:HG3	3	0.15	0.03	0.14
(3,585)	1:5:A:VAL:HG12	1:6:A:ARG:HG3	3	0.15	0.03	0.14
(3,585)	1:5:A:VAL:HG13	1:6:A:ARG:HG3	3	0.15	0.03	0.14
(1,387)	1:10:A:GLN:H	1:10:A:GLN:HE22	3	0.12	0.01	0.12
(3,354)	1:10:A:GLN:H	1:10:A:GLN:HE22	3	0.12	0.01	0.12
(1,158)	1:13:A:LYS:H	1:13:A:LYS:HB2	3	0.12	0.01	0.12
(1,158)	1:13:A:LYS:H	1:13:A:LYS:HB3	3	0.12	0.01	0.12
(3,137)	1:13:A:LYS:H	1:13:A:LYS:HB2	3	0.12	0.01	0.12
(3,137)	1:13:A:LYS:H	1:13:A:LYS:HB3	3	0.12	0.01	0.12
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG21	3	0.11	0.01	0.11
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG22	3	0.11	0.01	0.11
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG23	3	0.11	0.01	0.11
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG21	3	0.11	0.01	0.11
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG22	3	0.11	0.01	0.11
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG23	3	0.11	0.01	0.11
(1,662)	1:5:A:VAL:HA	1:8:A:TYR:H	3	0.11	0.0	0.11
(3,595)	1:5:A:VAL:HA	1:8:A:TYR:H	3	0.11	0.01	0.11
(1,660)	1:7:A:LEU:HD21	1:8:A:TYR:H	3	0.11	0.0	0.11
(1,660)	1:7:A:LEU:HD22	1:8:A:TYR:H	3	0.11	0.0	0.11
(1,660)	1:7:A:LEU:HD23	1:8:A:TYR:H	3	0.11	0.0	0.11
(3,593)	1:7:A:LEU:HD21	1:8:A:TYR:H	3	0.11	0.0	0.11
(3,593)	1:7:A:LEU:HD22	1:8:A:TYR:H	3	0.11	0.0	0.11
(3,593)	1:7:A:LEU:HD23	1:8:A:TYR:H	3	0.11	0.0	0.11
(1,220)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	2	0.66	0.02	0.66
(3,197)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	2	0.66	0.02	0.66
(1,221)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	2	0.44	0.01	0.44
(3,198)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	2	0.44	0.01	0.44
(1,39)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	2	0.3	0.1	0.3
(3,33)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	2	0.3	0.1	0.3
(1,331)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	2	0.3	0.01	0.3
(1,331)	1:11:A:TRP:HE1	1:21:A:ARG:HG3	2	0.3	0.01	0.3
(3,302)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	2	0.3	0.01	0.3
(3,302)	1:11:A:TRP:HE1	1:21:A:ARG:HG3	2	0.3	0.01	0.3
(1,129)	1:10:A:GLN:HA	1:10:A:GLN:HE21	2	0.16	0.04	0.16
(3,108)	1:10:A:GLN:HA	1:10:A:GLN:HE21	2	0.16	0.04	0.16
(1,32)	1:6:A:ARG:HA	1:6:A:ARG:HD3	2	0.12	0.01	0.12
(1,677)	1:9:A:ILE:HG21	1:13:A:LYS:HG3	2	0.12	0.0	0.12
(1,677)	1:9:A:ILE:HG22	1:13:A:LYS:HG3	2	0.12	0.0	0.12

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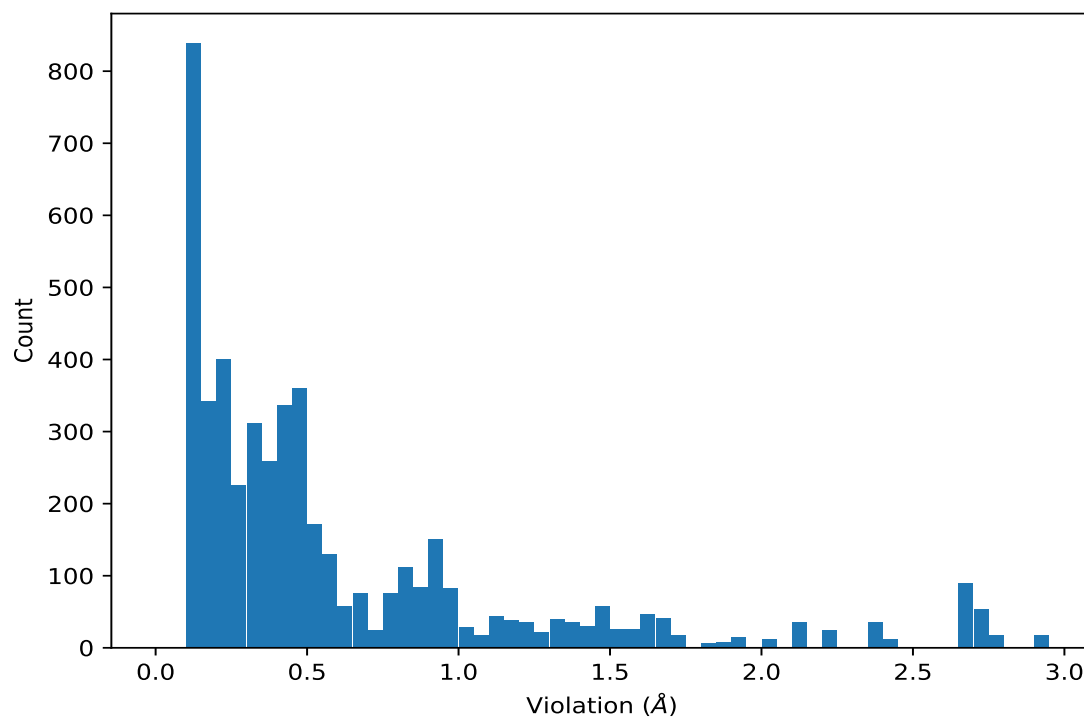
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,677)	1:9:A:ILE:HG23	1:13:A:LYS:HG3	2	0.12	0.0	0.12
(3,27)	1:6:A:ARG:HA	1:6:A:ARG:HD3	2	0.12	0.01	0.12
(3,605)	1:9:A:ILE:HG21	1:13:A:LYS:HG3	2	0.12	0.0	0.12
(3,605)	1:9:A:ILE:HG22	1:13:A:LYS:HG3	2	0.12	0.0	0.12
(3,605)	1:9:A:ILE:HG23	1:13:A:LYS:HG3	2	0.12	0.0	0.12
(1,312)	1:11:A:TRP:HD1	1:23:A:PRO:HA	2	0.12	0.0	0.12
(1,487)	1:10:A:GLN:H	1:11:A:TRP:HB3	2	0.12	0.0	0.12
(3,284)	1:11:A:TRP:HD1	1:23:A:PRO:HA	2	0.12	0.0	0.12
(3,438)	1:10:A:GLN:H	1:11:A:TRP:HB3	2	0.12	0.0	0.12
(1,663)	1:10:A:GLN:HA	1:13:A:LYS:H	2	0.11	0.0	0.11
(3,596)	1:10:A:GLN:HA	1:13:A:LYS:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	3	2.92
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	3	2.92
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	3	2.92
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	3	2.92
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	3	2.92
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	3	2.92
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	3	2.92
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	3	2.92
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	3	2.92
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	3	2.92
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	3	2.92
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	3	2.92
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	3	2.92
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	3	2.92
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	3	2.92
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	3	2.92
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	3	2.92
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	3	2.92
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	9	2.76
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	9	2.76
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	9	2.76
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	9	2.76
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	9	2.76
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	9	2.76
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	9	2.76
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	9	2.76
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	9	2.76
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	9	2.76
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	9	2.76
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	9	2.76
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	9	2.76
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	9	2.76
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	9	2.76
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	9	2.76
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	9	2.76
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	9	2.76
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	6	2.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	6	2.74
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	6	2.74
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	6	2.74
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	6	2.74
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	6	2.74
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	6	2.74
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	6	2.74
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	6	2.74
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	6	2.73
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	6	2.73
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	6	2.73
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	6	2.73
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	6	2.73
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	6	2.73
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	6	2.73
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	6	2.73
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	6	2.73
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	1	2.72
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	1	2.72
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	1	2.72
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	1	2.72
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	1	2.72
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	1	2.72
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	1	2.72
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	1	2.72
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	1	2.72
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	1	2.72
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	1	2.72
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	1	2.72
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	1	2.72
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	1	2.72
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	1	2.72
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	1	2.72
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	1	2.72
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	1	2.72
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	7	2.71
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	7	2.71
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	7	2.71
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	7	2.71
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	7	2.71
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	7	2.71
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	7	2.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	7	2.71
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	7	2.71
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	7	2.71
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	7	2.71
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	7	2.71
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	7	2.71
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	7	2.71
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	7	2.71
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	7	2.71
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	7	2.71
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	7	2.71
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	10	2.69
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	10	2.69
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	10	2.69
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	10	2.69
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	10	2.69
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	10	2.69
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	10	2.69
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	10	2.69
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	10	2.69
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	10	2.69
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	10	2.69
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	10	2.69
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	10	2.69
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	10	2.69
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	10	2.69
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	10	2.69
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	10	2.69
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	10	2.69
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	4	2.68
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	4	2.68
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	4	2.68
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	4	2.68
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	4	2.68
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	4	2.68
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	4	2.68
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	4	2.68
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	4	2.68
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	4	2.68
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	4	2.68
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	4	2.68
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	4	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	4	2.68
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	4	2.68
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	4	2.68
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	4	2.68
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	4	2.68
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	2	2.67
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	2	2.67
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	2	2.67
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	2	2.67
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	2	2.67
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	2	2.67
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	2	2.67
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	2	2.67
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	2	2.67
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	5	2.67
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	5	2.67
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	5	2.67
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	5	2.67
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	5	2.67
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	5	2.67
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	5	2.67
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	5	2.67
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	5	2.67
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	2	2.67
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	2	2.67
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	2	2.67
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	2	2.67
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	2	2.67
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	2	2.67
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	2	2.67
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	2	2.67
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	2	2.67
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	5	2.67
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	5	2.67
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	5	2.67
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	5	2.67
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	5	2.67
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	5	2.67
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	5	2.67
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	5	2.67
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	5	2.67
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	8	2.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	8	2.66
(4,73)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	8	2.66
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	8	2.66
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	8	2.66
(4,73)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	8	2.66
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	8	2.66
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	8	2.66
(4,73)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	8	2.66
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD21	8	2.66
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD22	8	2.66
(1,685)	1:9:A:ILE:HG21	1:12:A:LEU:HD23	8	2.66
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD21	8	2.66
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD22	8	2.66
(1,685)	1:9:A:ILE:HG22	1:12:A:LEU:HD23	8	2.66
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD21	8	2.66
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD22	8	2.66
(1,685)	1:9:A:ILE:HG23	1:12:A:LEU:HD23	8	2.66
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	1	2.44
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	1	2.44
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	1	2.44
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	1	2.44
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	1	2.44
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	1	2.44
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	1	2.44
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	1	2.44
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	1	2.44
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	1	2.44
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	1	2.44
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	1	2.44
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	2	2.4
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	2	2.4
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	2	2.4
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	2	2.4
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	2	2.4
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	2	2.4
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	2	2.4
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	2	2.4
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	2	2.4
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	2	2.4
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	2	2.4
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	2	2.4
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	3	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	3	2.39
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	3	2.39
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	3	2.39
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	3	2.39
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	3	2.39
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	3	2.39
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	3	2.39
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	3	2.39
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	3	2.39
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	3	2.39
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	3	2.39
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	5	2.37
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	5	2.37
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	5	2.37
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	5	2.37
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	5	2.37
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	5	2.37
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	5	2.37
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	5	2.37
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	5	2.37
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	5	2.37
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	5	2.37
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	5	2.37
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	6	2.22
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	6	2.22
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	6	2.22
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	6	2.22
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	6	2.22
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	6	2.22
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	6	2.22
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	6	2.22
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	6	2.22
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	6	2.22
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	6	2.22
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	6	2.22
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	8	2.21
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	8	2.21
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	8	2.21
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	8	2.21
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	8	2.21
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	8	2.21
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	8	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	8	2.21
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	8	2.21
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	8	2.21
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	8	2.21
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	8	2.21
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	10	2.12
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	10	2.12
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	10	2.12
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	10	2.12
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	10	2.12
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	10	2.12
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	10	2.12
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	10	2.12
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	10	2.12
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	10	2.12
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	10	2.12
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	10	2.12
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	7	2.11
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	7	2.11
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	7	2.11
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	7	2.11
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	7	2.11
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	7	2.11
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	7	2.11
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	7	2.11
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	7	2.11
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	7	2.11
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	7	2.11
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	7	2.11
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	4	2.1
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	4	2.1
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	4	2.1
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	4	2.1
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	4	2.1
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	4	2.1
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	4	2.1
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	4	2.1
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	4	2.1
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	4	2.1
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	4	2.1
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	4	2.1
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	9	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,29)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	9	2.01
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	9	2.01
(4,29)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	9	2.01
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	9	2.01
(4,29)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	9	2.01
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE1	9	2.01
(1,320)	1:4:A:ALA:HB1	1:8:A:TYR:HE2	9	2.01
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE1	9	2.01
(1,320)	1:4:A:ALA:HB2	1:8:A:TYR:HE2	9	2.01
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE1	9	2.01
(1,320)	1:4:A:ALA:HB3	1:8:A:TYR:HE2	9	2.01
(3,603)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	8	1.95
(1,674)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	1	1.95
(1,674)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	8	1.95
(3,603)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	1	1.94
(3,603)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	2	1.93
(1,674)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	2	1.93
(3,603)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	5	1.92
(1,674)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	5	1.92
(4,64)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	4	1.91
(4,64)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	4	1.91
(4,64)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	4	1.91
(1,648)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	4	1.91
(1,648)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	4	1.91
(1,648)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	4	1.91
(3,603)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	7	1.9
(1,674)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	7	1.9
(4,74)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	7	1.85
(4,74)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	7	1.85
(4,74)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	7	1.85
(1,688)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	7	1.85
(1,688)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	7	1.85
(1,688)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	7	1.85
(4,64)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	3	1.83
(4,64)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	3	1.83
(4,64)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	3	1.83
(1,648)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	3	1.83
(1,648)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	3	1.83
(1,648)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	3	1.83
(4,51)	1:2:A:GLU:HA	1:5:A:VAL:HB	2	1.74
(1,527)	1:2:A:GLU:HA	1:5:A:VAL:HB	2	1.74
(4,74)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	8	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,74)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	8	1.73
(4,74)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	8	1.73
(1,688)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	8	1.73
(1,688)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	8	1.73
(1,688)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	8	1.73
(4,74)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	5	1.72
(4,74)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	5	1.72
(4,74)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	5	1.72
(4,51)	1:2:A:GLU:HA	1:5:A:VAL:HB	6	1.72
(1,688)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	5	1.72
(1,688)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	5	1.72
(1,688)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	5	1.72
(1,527)	1:2:A:GLU:HA	1:5:A:VAL:HB	6	1.72
(4,51)	1:2:A:GLU:HA	1:5:A:VAL:HB	1	1.71
(1,527)	1:2:A:GLU:HA	1:5:A:VAL:HB	1	1.71
(4,74)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	4	1.7
(4,74)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	4	1.7
(4,74)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	4	1.7
(4,64)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	8	1.7
(4,64)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	8	1.7
(4,64)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	8	1.7
(4,51)	1:2:A:GLU:HA	1:5:A:VAL:HB	5	1.7
(1,688)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	4	1.7
(1,688)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	4	1.7
(1,688)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	4	1.7
(1,648)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	8	1.7
(1,648)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	8	1.7
(1,648)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	8	1.7
(1,527)	1:2:A:GLU:HA	1:5:A:VAL:HB	5	1.7
(4,64)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	5	1.69
(4,64)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	5	1.69
(4,64)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	5	1.69
(4,51)	1:2:A:GLU:HA	1:5:A:VAL:HB	3	1.69
(1,648)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	5	1.69
(1,648)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	5	1.69
(1,648)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	5	1.69
(1,527)	1:2:A:GLU:HA	1:5:A:VAL:HB	3	1.69
(4,64)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	6	1.68
(4,64)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	6	1.68
(4,64)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	6	1.68
(4,64)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	7	1.68
(4,64)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	7	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,64)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	7	1.68
(4,51)	1:2:A:GLU:HA	1:5:A:VAL:HB	7	1.68
(4,51)	1:2:A:GLU:HA	1:5:A:VAL:HB	8	1.68
(1,648)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	6	1.68
(1,648)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	6	1.68
(1,648)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	6	1.68
(1,648)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	7	1.68
(1,648)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	7	1.68
(1,648)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	7	1.68
(1,527)	1:2:A:GLU:HA	1:5:A:VAL:HB	7	1.68
(1,527)	1:2:A:GLU:HA	1:5:A:VAL:HB	8	1.68
(1,688)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	1	1.66
(1,688)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	1	1.66
(1,688)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	1	1.66
(4,74)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	1	1.65
(4,74)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	1	1.65
(4,74)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	1	1.65
(4,74)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	2	1.65
(4,74)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	2	1.65
(4,74)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	2	1.65
(4,65)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	9	1.65
(4,65)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	9	1.65
(4,65)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	9	1.65
(1,688)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	2	1.65
(1,688)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	2	1.65
(1,688)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	2	1.65
(1,651)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	9	1.65
(1,651)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	9	1.65
(1,651)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	9	1.65
(3,603)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	4	1.64
(1,674)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	4	1.64
(4,65)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	6	1.63
(4,65)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	6	1.63
(4,65)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	6	1.63
(1,651)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	6	1.63
(1,651)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	6	1.63
(1,651)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	6	1.63
(4,74)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	3	1.61
(4,74)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	3	1.61
(4,74)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	3	1.61
(4,74)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	10	1.61
(4,74)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	10	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,74)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	10	1.61
(1,688)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	3	1.61
(1,688)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	3	1.61
(1,688)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	3	1.61
(1,688)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	10	1.61
(1,688)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	10	1.61
(1,688)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	10	1.61
(4,65)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	7	1.6
(4,65)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	7	1.6
(4,65)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	7	1.6
(4,51)	1:2:A:GLU:HA	1:5:A:VAL:HB	4	1.6
(4,51)	1:2:A:GLU:HA	1:5:A:VAL:HB	9	1.6
(4,51)	1:2:A:GLU:HA	1:5:A:VAL:HB	10	1.6
(1,651)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	7	1.6
(1,651)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	7	1.6
(1,651)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	7	1.6
(1,527)	1:2:A:GLU:HA	1:5:A:VAL:HB	4	1.6
(1,527)	1:2:A:GLU:HA	1:5:A:VAL:HB	9	1.6
(1,527)	1:2:A:GLU:HA	1:5:A:VAL:HB	10	1.6
(3,510)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	3	1.59
(1,566)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	3	1.59
(3,510)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	9	1.58
(1,566)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	9	1.58
(3,510)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	6	1.57
(1,566)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	6	1.57
(4,65)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	2	1.56
(4,65)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	2	1.56
(4,65)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	2	1.56
(4,65)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	5	1.56
(4,65)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	5	1.56
(4,65)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	5	1.56
(3,510)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	10	1.56
(1,651)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	2	1.56
(1,651)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	2	1.56
(1,651)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	2	1.56
(1,651)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	5	1.56
(1,651)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	5	1.56
(1,651)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	5	1.56
(1,566)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	10	1.56
(4,65)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	8	1.55
(4,65)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	8	1.55
(4,65)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	8	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,651)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	8	1.55
(1,651)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	8	1.55
(1,651)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	8	1.55
(4,65)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	1	1.54
(4,65)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	1	1.54
(4,65)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	1	1.54
(4,39)	1:1:A:GLU:HG2	1:4:A:ALA:H	4	1.54
(4,39)	1:1:A:GLU:HG3	1:4:A:ALA:H	4	1.54
(3,601)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	8	1.54
(1,672)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	8	1.54
(1,651)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	1	1.54
(1,651)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	1	1.54
(1,651)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	1	1.54
(1,424)	1:1:A:GLU:HG2	1:4:A:ALA:H	4	1.54
(1,424)	1:1:A:GLU:HG3	1:4:A:ALA:H	4	1.54
(3,601)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	1	1.53
(3,601)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	2	1.53
(3,601)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	5	1.53
(3,601)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	7	1.53
(1,672)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	1	1.53
(1,672)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	2	1.53
(1,672)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	5	1.53
(1,672)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	7	1.53
(4,64)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	10	1.5
(4,64)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	10	1.5
(4,64)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	10	1.5
(1,648)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	10	1.5
(1,648)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	10	1.5
(1,648)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	10	1.5
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	1.49
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	1.49
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	1.49
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	1.49
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	1.49
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	1.49
(4,74)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	9	1.48
(4,74)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	9	1.48
(4,74)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	9	1.48
(1,688)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	9	1.48
(1,688)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	9	1.48
(1,688)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	9	1.48
(4,39)	1:1:A:GLU:HG2	1:4:A:ALA:H	10	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,39)	1:1:A:GLU:HG3	1:4:A:ALA:H	10	1.47
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	1.47
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	1.47
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	1.47
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	1.47
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	1.47
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	1.47
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	1.47
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	1.47
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	1.47
(1,424)	1:1:A:GLU:HG2	1:4:A:ALA:H	10	1.47
(1,424)	1:1:A:GLU:HG3	1:4:A:ALA:H	10	1.47
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	1.47
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	1.47
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	1.47
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	1.47
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	1.47
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	1.47
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	1.47
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	1.47
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	1.47
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	8	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	8	1.46
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	8	1.46
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	1.45
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	1.45
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	1.45
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	1.45
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	1.45
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	1.45
(4,64)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	2	1.44
(4,64)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	2	1.44
(4,64)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	2	1.44
(4,59)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	9	1.44
(4,59)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	9	1.44
(4,59)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	9	1.44
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	1.44
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	1.44
(4,14)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	1.44
(1,648)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	2	1.44
(1,648)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	2	1.44
(1,648)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	2	1.44
(1,598)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	9	1.44
(1,598)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	9	1.44
(1,598)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	9	1.44
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	1.44
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	1.44
(1,76)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	1.44
(4,59)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	2	1.42
(4,59)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	2	1.42
(4,59)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	2	1.42
(1,598)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	2	1.42
(1,598)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	2	1.42
(1,598)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	2	1.42
(4,65)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	10	1.4
(4,65)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	10	1.4
(4,65)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	10	1.4
(3,325)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	10	1.4
(1,651)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	10	1.4
(1,651)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	10	1.4
(1,651)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	10	1.4
(1,356)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	10	1.4
(3,326)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	10	1.39
(4,65)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	4	1.38
(4,65)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	4	1.38
(4,65)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	4	1.38
(3,325)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	5	1.38
(1,651)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	4	1.38
(1,651)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	4	1.38
(1,651)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	4	1.38
(1,356)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	5	1.38
(4,37)	1:10:A:GLN:H	1:13:A:LYS:H	8	1.37
(3,601)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	4	1.37
(1,672)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	4	1.37
(1,406)	1:10:A:GLN:H	1:13:A:LYS:H	8	1.37
(4,74)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	6	1.36
(4,74)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	6	1.36
(4,74)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	6	1.36
(4,37)	1:10:A:GLN:H	1:13:A:LYS:H	7	1.36
(3,326)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	5	1.36
(1,688)	1:7:A:LEU:HD21	1:24:A:PRO:HG3	6	1.36
(1,688)	1:7:A:LEU:HD22	1:24:A:PRO:HG3	6	1.36
(1,688)	1:7:A:LEU:HD23	1:24:A:PRO:HG3	6	1.36
(1,406)	1:10:A:GLN:H	1:13:A:LYS:H	7	1.36
(1,357)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	5	1.36
(3,603)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	3	1.35
(3,326)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	9	1.35
(1,674)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	3	1.35
(1,357)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	9	1.35
(4,39)	1:1:A:GLU:HG2	1:4:A:ALA:H	3	1.34
(4,39)	1:1:A:GLU:HG3	1:4:A:ALA:H	3	1.34
(4,37)	1:10:A:GLN:H	1:13:A:LYS:H	3	1.34
(3,326)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	2	1.34
(3,326)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	6	1.34
(1,424)	1:1:A:GLU:HG2	1:4:A:ALA:H	3	1.34
(1,424)	1:1:A:GLU:HG3	1:4:A:ALA:H	3	1.34
(1,406)	1:10:A:GLN:H	1:13:A:LYS:H	3	1.34
(1,357)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	2	1.34
(1,357)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	6	1.34
(4,37)	1:10:A:GLN:H	1:13:A:LYS:H	10	1.33
(3,326)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	1	1.33
(3,325)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	6	1.33
(1,406)	1:10:A:GLN:H	1:13:A:LYS:H	10	1.33
(1,357)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	1	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	6	1.33
(4,37)	1:10:A:GLN:H	1:13:A:LYS:H	5	1.32
(3,326)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	3	1.32
(1,406)	1:10:A:GLN:H	1:13:A:LYS:H	5	1.32
(1,357)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	3	1.32
(4,37)	1:10:A:GLN:H	1:13:A:LYS:H	4	1.31
(4,37)	1:10:A:GLN:H	1:13:A:LYS:H	6	1.31
(3,326)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	4	1.31
(3,326)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	8	1.31
(1,406)	1:10:A:GLN:H	1:13:A:LYS:H	4	1.31
(1,406)	1:10:A:GLN:H	1:13:A:LYS:H	6	1.31
(1,357)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	4	1.31
(1,357)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	8	1.31
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	1	1.3
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	1	1.3
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	1	1.3
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	1	1.3
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	1	1.3
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	1	1.3
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	1	1.3
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	1	1.3
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	1	1.3
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	1	1.3
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	1	1.3
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	1	1.3
(4,37)	1:10:A:GLN:H	1:13:A:LYS:H	1	1.29
(3,325)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	4	1.29
(1,406)	1:10:A:GLN:H	1:13:A:LYS:H	1	1.29
(1,356)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	4	1.29
(4,65)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	3	1.28
(4,65)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	3	1.28
(4,65)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	3	1.28
(1,651)	1:5:A:VAL:HG11	1:9:A:ILE:HG12	3	1.28
(1,651)	1:5:A:VAL:HG12	1:9:A:ILE:HG12	3	1.28
(1,651)	1:5:A:VAL:HG13	1:9:A:ILE:HG12	3	1.28
(4,37)	1:10:A:GLN:H	1:13:A:LYS:H	2	1.27
(3,325)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	3	1.27
(3,325)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	9	1.27
(1,406)	1:10:A:GLN:H	1:13:A:LYS:H	2	1.27
(1,356)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	3	1.27
(1,356)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	9	1.27
(4,37)	1:10:A:GLN:H	1:13:A:LYS:H	9	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,603)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	10	1.26
(1,674)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	10	1.26
(1,406)	1:10:A:GLN:H	1:13:A:LYS:H	9	1.26
(4,53)	1:3:A:GLU:HA	1:6:A:ARG:HB2	10	1.25
(1,534)	1:3:A:GLU:HA	1:6:A:ARG:HB2	10	1.25
(4,59)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	4	1.24
(4,59)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	4	1.24
(4,59)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	4	1.24
(4,59)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	7	1.24
(4,59)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	7	1.24
(4,59)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	7	1.24
(3,326)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	7	1.24
(3,325)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	2	1.24
(1,598)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	4	1.24
(1,598)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	4	1.24
(1,598)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	4	1.24
(1,598)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	7	1.24
(1,598)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	7	1.24
(1,598)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	7	1.24
(1,357)	1:11:A:TRP:HZ2	1:23:A:PRO:HG2	7	1.24
(1,356)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	2	1.24
(3,325)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	1	1.23
(1,356)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	1	1.23
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	7	1.22
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	7	1.22
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	7	1.22
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	7	1.22
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	7	1.22
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	7	1.22
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	7	1.22
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	7	1.22
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	7	1.22
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	7	1.22
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	7	1.22
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	7	1.22
(4,59)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	8	1.21
(4,59)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	8	1.21
(4,59)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	8	1.21
(1,598)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	8	1.21
(1,598)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	8	1.21
(1,598)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	8	1.21
(4,64)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	1	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,64)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	1	1.2
(4,64)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	1	1.2
(4,59)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	1	1.2
(4,59)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	1	1.2
(4,59)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	1	1.2
(1,648)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	1	1.2
(1,648)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	1	1.2
(1,648)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	1	1.2
(1,598)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	1	1.2
(1,598)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	1	1.2
(1,598)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	1	1.2
(4,59)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	5	1.17
(4,59)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	5	1.17
(4,59)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	5	1.17
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	8	1.17
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	8	1.17
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	8	1.17
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	8	1.17
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	8	1.17
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	8	1.17
(1,598)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	5	1.17
(1,598)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	5	1.17
(1,598)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	5	1.17
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	8	1.17
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	8	1.17
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	8	1.17
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	8	1.17
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	8	1.17
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	8	1.17
(4,59)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	6	1.16
(4,59)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	6	1.16
(4,59)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	6	1.16
(4,53)	1:3:A:GLU:HA	1:6:A:ARG:HB2	4	1.16
(1,598)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	6	1.16
(1,598)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	6	1.16
(1,598)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	6	1.16
(1,534)	1:3:A:GLU:HA	1:6:A:ARG:HB2	4	1.16
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	2	1.15
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	2	1.15
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	2	1.15
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	2	1.15
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	2	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	2	1.15
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	5	1.15
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	5	1.15
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	5	1.15
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	5	1.15
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	5	1.15
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	5	1.15
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	2	1.15
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	2	1.15
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	2	1.15
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	2	1.15
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	2	1.15
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	2	1.15
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	5	1.15
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	5	1.15
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	5	1.15
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	5	1.15
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	5	1.15
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	5	1.15
(4,32)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	1.12
(3,510)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	4	1.12
(1,566)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	4	1.12
(1,380)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	4	1.12
(4,59)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	3	1.11
(4,59)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	3	1.11
(4,59)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	3	1.11
(4,59)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	10	1.11
(4,59)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	10	1.11
(4,59)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	10	1.11
(1,598)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	3	1.11
(1,598)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	3	1.11
(1,598)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	3	1.11
(1,598)	1:7:A:LEU:HD21	1:10:A:GLN:HB3	10	1.11
(1,598)	1:7:A:LEU:HD22	1:10:A:GLN:HB3	10	1.11
(1,598)	1:7:A:LEU:HD23	1:10:A:GLN:HB3	10	1.11
(3,603)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	9	1.1
(3,510)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	1	1.1
(1,674)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	9	1.1
(1,566)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	1	1.1
(3,603)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	6	1.08
(1,674)	1:7:A:LEU:HB3	1:24:A:PRO:HB3	6	1.08
(3,510)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	2	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	2	1.07
(3,601)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	10	1.06
(3,510)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	5	1.06
(1,672)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	10	1.06
(1,566)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	5	1.06
(4,32)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	1.05
(4,32)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	1.05
(4,32)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	1.05
(4,32)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	1.05
(3,510)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	8	1.05
(1,566)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	8	1.05
(1,380)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	2	1.05
(1,380)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	3	1.05
(1,380)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	5	1.05
(1,380)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	6	1.05
(4,32)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	1.04
(1,380)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	1	1.04
(1,380)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	1.04
(4,32)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	1.03
(4,32)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	1.03
(4,32)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	9	1.03
(4,32)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.03
(3,510)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	7	1.03
(1,566)	1:7:A:LEU:HB3	1:24:A:PRO:HB2	7	1.03
(1,380)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	7	1.03
(1,380)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	8	1.03
(1,380)	1:11:A:TRP:HB2	1:11:A:TRP:HZ3	10	1.03
(3,614)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	2	1.02
(3,614)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	2	1.02
(3,614)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	2	1.02
(1,689)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	2	1.02
(1,689)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	2	1.02
(1,689)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	2	1.02
(3,614)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	5	1.0
(3,614)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	5	1.0
(3,614)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	5	1.0
(3,601)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	3	1.0
(3,601)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	6	1.0
(1,689)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	5	1.0
(1,689)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	5	1.0
(1,689)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	5	1.0
(1,672)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	3	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	6	1.0
(4,72)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	6	0.99
(4,72)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	6	0.99
(4,72)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	6	0.99
(3,380)	1:2:A:GLU:HG2	1:3:A:GLU:H	6	0.99
(1,681)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	6	0.99
(1,681)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	6	0.99
(1,681)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	6	0.99
(1,418)	1:2:A:GLU:HG2	1:3:A:GLU:H	6	0.99
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	4	0.97
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	4	0.97
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	4	0.97
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	4	0.97
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	4	0.97
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	4	0.97
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	4	0.97
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	4	0.97
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	4	0.97
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	4	0.97
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	4	0.97
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	4	0.97
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	4	0.97
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	4	0.97
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	4	0.97
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	4	0.97
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	4	0.97
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	4	0.97
(4,72)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	7	0.96
(4,72)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	7	0.96
(4,72)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	7	0.96
(4,72)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	10	0.96
(4,72)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	10	0.96
(4,72)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	10	0.96
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.96
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.96
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.96
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.96
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.96
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.96
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.96
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.96
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	1	0.96
(4,35)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	2	0.96
(4,35)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	4	0.96
(4,35)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	5	0.96
(4,35)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	6	0.96
(4,35)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	10	0.96
(3,614)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	4	0.96
(3,614)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	4	0.96
(3,614)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	4	0.96
(3,614)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	8	0.96
(3,614)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	8	0.96
(3,614)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	8	0.96
(3,325)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	8	0.96
(1,689)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	4	0.96
(1,689)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	4	0.96
(1,689)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	4	0.96
(1,689)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	8	0.96
(1,689)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	8	0.96
(1,689)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	8	0.96
(1,681)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	7	0.96
(1,681)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	7	0.96
(1,681)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	7	0.96
(1,681)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	10	0.96
(1,681)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	10	0.96
(1,681)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	10	0.96
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.96
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.96
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.96
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.96
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.96
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.96
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.96
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.96
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.96
(1,396)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	1	0.96
(1,396)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	2	0.96
(1,396)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	4	0.96
(1,396)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	5	0.96
(1,396)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	6	0.96
(1,396)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	10	0.96
(1,356)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	8	0.96
(4,72)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	3	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,72)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	3	0.95
(4,72)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	3	0.95
(4,72)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	8	0.95
(4,72)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	8	0.95
(4,72)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	8	0.95
(4,35)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	3	0.95
(4,35)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	7	0.95
(4,35)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	8	0.95
(4,35)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	9	0.95
(1,681)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	3	0.95
(1,681)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	3	0.95
(1,681)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	3	0.95
(1,681)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	8	0.95
(1,681)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	8	0.95
(1,681)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	8	0.95
(1,396)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	3	0.95
(1,396)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	7	0.95
(1,396)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	8	0.95
(1,396)	1:11:A:TRP:HE3	1:11:A:TRP:HZ2	9	0.95
(4,72)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	4	0.94
(4,72)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	4	0.94
(4,72)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	4	0.94
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	5	0.94
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	5	0.94
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	5	0.94
(4,53)	1:3:A:GLU:HA	1:6:A:ARG:HB2	9	0.94
(3,380)	1:2:A:GLU:HG2	1:3:A:GLU:H	5	0.94
(3,380)	1:2:A:GLU:HG2	1:3:A:GLU:H	8	0.94
(3,325)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	7	0.94
(3,322)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.94
(1,681)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	4	0.94
(1,681)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	4	0.94
(1,681)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	4	0.94
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	5	0.94
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	5	0.94
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	5	0.94
(1,534)	1:3:A:GLU:HA	1:6:A:ARG:HB2	9	0.94
(1,418)	1:2:A:GLU:HG2	1:3:A:GLU:H	5	0.94
(1,418)	1:2:A:GLU:HG2	1:3:A:GLU:H	8	0.94
(1,356)	1:11:A:TRP:HH2	1:23:A:PRO:HG2	7	0.94
(1,353)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.94
(4,72)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	5	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,72)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	5	0.93
(4,72)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	5	0.93
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	7	0.93
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	7	0.93
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	7	0.93
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	8	0.93
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	8	0.93
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	8	0.93
(3,614)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	1	0.93
(3,614)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	1	0.93
(3,614)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	1	0.93
(3,601)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	9	0.93
(3,417)	1:8:A:TYR:H	1:24:A:PRO:HB3	2	0.93
(1,689)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	1	0.93
(1,689)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	1	0.93
(1,689)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	1	0.93
(1,681)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	5	0.93
(1,681)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	5	0.93
(1,681)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	5	0.93
(1,672)	1:8:A:TYR:HB3	1:24:A:PRO:HB3	9	0.93
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	7	0.93
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	7	0.93
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	7	0.93
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	8	0.93
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	8	0.93
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	8	0.93
(1,459)	1:8:A:TYR:H	1:24:A:PRO:HB3	2	0.93
(4,72)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	1	0.92
(4,72)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	1	0.92
(4,72)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	1	0.92
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	9	0.92
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	9	0.92
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	9	0.92
(3,560)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	8	0.92
(3,417)	1:8:A:TYR:H	1:24:A:PRO:HB3	8	0.92
(3,322)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	7	0.92
(1,681)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	1	0.92
(1,681)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	1	0.92
(1,681)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	1	0.92
(1,623)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	8	0.92
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	9	0.92
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	9	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	9	0.92
(1,459)	1:8:A:TYR:H	1:24:A:PRO:HB3	8	0.92
(1,353)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	7	0.92
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	1	0.91
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	1	0.91
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	1	0.91
(4,46)	1:7:A:LEU:HD11	1:10:A:GLN:H	3	0.91
(4,46)	1:7:A:LEU:HD12	1:10:A:GLN:H	3	0.91
(4,46)	1:7:A:LEU:HD13	1:10:A:GLN:H	3	0.91
(3,614)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	10	0.91
(3,614)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	10	0.91
(3,614)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	10	0.91
(3,417)	1:8:A:TYR:H	1:24:A:PRO:HB3	1	0.91
(3,380)	1:2:A:GLU:HG2	1:3:A:GLU:H	1	0.91
(1,689)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	10	0.91
(1,689)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	10	0.91
(1,689)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	10	0.91
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	1	0.91
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	1	0.91
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	1	0.91
(1,469)	1:7:A:LEU:HD11	1:10:A:GLN:H	3	0.91
(1,469)	1:7:A:LEU:HD12	1:10:A:GLN:H	3	0.91
(1,469)	1:7:A:LEU:HD13	1:10:A:GLN:H	3	0.91
(1,459)	1:8:A:TYR:H	1:24:A:PRO:HB3	1	0.91
(1,418)	1:2:A:GLU:HG2	1:3:A:GLU:H	1	0.91
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	2	0.9
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	2	0.9
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	2	0.9
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.9
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.9
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.9
(3,614)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	3	0.9
(3,614)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	3	0.9
(3,614)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	3	0.9
(3,614)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	7	0.9
(3,614)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	7	0.9
(3,614)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	7	0.9
(3,560)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	9	0.9
(3,473)	1:11:A:TRP:HA	1:14:A:ASP:HB3	6	0.9
(3,417)	1:8:A:TYR:H	1:24:A:PRO:HB3	5	0.9
(3,380)	1:2:A:GLU:HG2	1:3:A:GLU:H	2	0.9
(3,322)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	5	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,322)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	6	0.9
(3,322)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	9	0.9
(3,322)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	10	0.9
(1,689)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	3	0.9
(1,689)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	3	0.9
(1,689)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	3	0.9
(1,689)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	7	0.9
(1,689)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	7	0.9
(1,689)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	7	0.9
(1,623)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	9	0.9
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	2	0.9
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	2	0.9
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	2	0.9
(1,523)	1:11:A:TRP:HA	1:14:A:ASP:HB3	6	0.9
(1,459)	1:8:A:TYR:H	1:24:A:PRO:HB3	5	0.9
(1,418)	1:2:A:GLU:HG2	1:3:A:GLU:H	2	0.9
(1,353)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	5	0.9
(1,353)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	6	0.9
(1,353)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	9	0.9
(1,353)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	10	0.9
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG21	10	0.9
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG22	10	0.9
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG23	10	0.9
(4,72)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	9	0.89
(4,72)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	9	0.89
(4,72)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	9	0.89
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	3	0.89
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	3	0.89
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	3	0.89
(4,48)	1:5:A:VAL:HB	1:6:A:ARG:H	9	0.89
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG21	4	0.89
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG22	4	0.89
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG23	4	0.89
(1,681)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	9	0.89
(1,681)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	9	0.89
(1,681)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	9	0.89
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	3	0.89
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	3	0.89
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	3	0.89
(1,483)	1:5:A:VAL:HB	1:6:A:ARG:H	9	0.89
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG21	4	0.89
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG22	4	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG23	4	0.89
(3,380)	1:2:A:GLU:HG2	1:3:A:GLU:H	9	0.88
(3,322)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	1	0.88
(1,418)	1:2:A:GLU:HG2	1:3:A:GLU:H	9	0.88
(1,353)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	1	0.88
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	3	0.87
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	3	0.87
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	3	0.87
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	3	0.87
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	3	0.87
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	3	0.87
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	3	0.87
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	3	0.87
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	3	0.87
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG21	1	0.87
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG22	1	0.87
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG23	1	0.87
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG21	7	0.87
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG22	7	0.87
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG23	7	0.87
(3,417)	1:8:A:TYR:H	1:24:A:PRO:HB3	7	0.87
(3,322)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	3	0.87
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	3	0.87
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	3	0.87
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	3	0.87
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	3	0.87
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	3	0.87
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	3	0.87
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	3	0.87
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	3	0.87
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	3	0.87
(1,459)	1:8:A:TYR:H	1:24:A:PRO:HB3	7	0.87
(1,353)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	3	0.87
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG21	1	0.87
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG22	1	0.87
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG23	1	0.87
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG21	7	0.87
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG22	7	0.87
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG23	7	0.87
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG21	3	0.86
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG22	3	0.86
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG23	3	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG21	5	0.86
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG22	5	0.86
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG23	5	0.86
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG21	8	0.86
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG22	8	0.86
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG23	8	0.86
(3,473)	1:11:A:TRP:HA	1:14:A:ASP:HB3	1	0.86
(3,473)	1:11:A:TRP:HA	1:14:A:ASP:HB3	3	0.86
(3,473)	1:11:A:TRP:HA	1:14:A:ASP:HB3	8	0.86
(3,322)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	4	0.86
(1,523)	1:11:A:TRP:HA	1:14:A:ASP:HB3	1	0.86
(1,523)	1:11:A:TRP:HA	1:14:A:ASP:HB3	3	0.86
(1,523)	1:11:A:TRP:HA	1:14:A:ASP:HB3	8	0.86
(1,353)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	4	0.86
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG21	3	0.86
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG22	3	0.86
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG23	3	0.86
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG21	5	0.86
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG22	5	0.86
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG23	5	0.86
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG21	8	0.86
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG22	8	0.86
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG23	8	0.86
(4,48)	1:5:A:VAL:HB	1:6:A:ARG:H	1	0.85
(4,48)	1:5:A:VAL:HB	1:6:A:ARG:H	6	0.85
(4,46)	1:7:A:LEU:HD11	1:10:A:GLN:H	4	0.85
(4,46)	1:7:A:LEU:HD12	1:10:A:GLN:H	4	0.85
(4,46)	1:7:A:LEU:HD13	1:10:A:GLN:H	4	0.85
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG21	2	0.85
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG22	2	0.85
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG23	2	0.85
(3,560)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	7	0.85
(3,473)	1:11:A:TRP:HA	1:14:A:ASP:HB3	4	0.85
(3,473)	1:11:A:TRP:HA	1:14:A:ASP:HB3	5	0.85
(3,473)	1:11:A:TRP:HA	1:14:A:ASP:HB3	7	0.85
(3,473)	1:11:A:TRP:HA	1:14:A:ASP:HB3	10	0.85
(1,623)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	7	0.85
(1,523)	1:11:A:TRP:HA	1:14:A:ASP:HB3	4	0.85
(1,523)	1:11:A:TRP:HA	1:14:A:ASP:HB3	5	0.85
(1,523)	1:11:A:TRP:HA	1:14:A:ASP:HB3	7	0.85
(1,523)	1:11:A:TRP:HA	1:14:A:ASP:HB3	10	0.85
(1,483)	1:5:A:VAL:HB	1:6:A:ARG:H	1	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:5:A:VAL:HB	1:6:A:ARG:H	6	0.85
(1,469)	1:7:A:LEU:HD11	1:10:A:GLN:H	4	0.85
(1,469)	1:7:A:LEU:HD12	1:10:A:GLN:H	4	0.85
(1,469)	1:7:A:LEU:HD13	1:10:A:GLN:H	4	0.85
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG21	2	0.85
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG22	2	0.85
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG23	2	0.85
(4,48)	1:5:A:VAL:HB	1:6:A:ARG:H	2	0.84
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG21	9	0.84
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG22	9	0.84
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG23	9	0.84
(3,614)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	9	0.84
(3,614)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	9	0.84
(3,614)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	9	0.84
(1,689)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	9	0.84
(1,689)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	9	0.84
(1,689)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	9	0.84
(1,483)	1:5:A:VAL:HB	1:6:A:ARG:H	2	0.84
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG21	9	0.84
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG22	9	0.84
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG23	9	0.84
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	4	0.83
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	4	0.83
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	4	0.83
(4,48)	1:5:A:VAL:HB	1:6:A:ARG:H	7	0.83
(4,48)	1:5:A:VAL:HB	1:6:A:ARG:H	8	0.83
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG21	6	0.83
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG22	6	0.83
(4,5)	1:5:A:VAL:H	1:5:A:VAL:HG23	6	0.83
(3,473)	1:11:A:TRP:HA	1:14:A:ASP:HB3	9	0.83
(3,322)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	2	0.83
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	4	0.83
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	4	0.83
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	4	0.83
(1,523)	1:11:A:TRP:HA	1:14:A:ASP:HB3	9	0.83
(1,483)	1:5:A:VAL:HB	1:6:A:ARG:H	7	0.83
(1,483)	1:5:A:VAL:HB	1:6:A:ARG:H	8	0.83
(1,353)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	2	0.83
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG21	6	0.83
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG22	6	0.83
(1,28)	1:5:A:VAL:H	1:5:A:VAL:HG23	6	0.83
(4,48)	1:5:A:VAL:HB	1:6:A:ARG:H	5	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,614)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	6	0.82
(3,614)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	6	0.82
(3,614)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	6	0.82
(3,586)	1:6:A:ARG:HG3	1:7:A:LEU:HD21	6	0.82
(3,586)	1:6:A:ARG:HG3	1:7:A:LEU:HD22	6	0.82
(3,586)	1:6:A:ARG:HG3	1:7:A:LEU:HD23	6	0.82
(3,575)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	0.82
(3,575)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	0.82
(1,689)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	6	0.82
(1,689)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	6	0.82
(1,689)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	6	0.82
(1,650)	1:6:A:ARG:HG3	1:7:A:LEU:HD21	6	0.82
(1,650)	1:6:A:ARG:HG3	1:7:A:LEU:HD22	6	0.82
(1,650)	1:6:A:ARG:HG3	1:7:A:LEU:HD23	6	0.82
(1,638)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	0.82
(1,638)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	0.82
(1,483)	1:5:A:VAL:HB	1:6:A:ARG:H	5	0.82
(4,46)	1:7:A:LEU:HD11	1:10:A:GLN:H	6	0.81
(4,46)	1:7:A:LEU:HD12	1:10:A:GLN:H	6	0.81
(4,46)	1:7:A:LEU:HD13	1:10:A:GLN:H	6	0.81
(4,46)	1:7:A:LEU:HD11	1:10:A:GLN:H	8	0.81
(4,46)	1:7:A:LEU:HD12	1:10:A:GLN:H	8	0.81
(4,46)	1:7:A:LEU:HD13	1:10:A:GLN:H	8	0.81
(3,575)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	0.81
(3,560)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	6	0.81
(3,473)	1:11:A:TRP:HA	1:14:A:ASP:HB3	2	0.81
(3,380)	1:2:A:GLU:HG2	1:3:A:GLU:H	7	0.81
(1,638)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	0.81
(1,623)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	6	0.81
(1,523)	1:11:A:TRP:HA	1:14:A:ASP:HB3	2	0.81
(1,469)	1:7:A:LEU:HD11	1:10:A:GLN:H	6	0.81
(1,469)	1:7:A:LEU:HD12	1:10:A:GLN:H	6	0.81
(1,469)	1:7:A:LEU:HD13	1:10:A:GLN:H	6	0.81
(1,469)	1:7:A:LEU:HD11	1:10:A:GLN:H	8	0.81
(1,469)	1:7:A:LEU:HD12	1:10:A:GLN:H	8	0.81
(1,469)	1:7:A:LEU:HD13	1:10:A:GLN:H	8	0.81
(1,418)	1:2:A:GLU:HG2	1:3:A:GLU:H	7	0.81
(4,46)	1:7:A:LEU:HD11	1:10:A:GLN:H	7	0.8
(4,46)	1:7:A:LEU:HD12	1:10:A:GLN:H	7	0.8
(4,46)	1:7:A:LEU:HD13	1:10:A:GLN:H	7	0.8
(4,46)	1:7:A:LEU:HD11	1:10:A:GLN:H	10	0.8
(4,46)	1:7:A:LEU:HD12	1:10:A:GLN:H	10	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,46)	1:7:A:LEU:HD13	1:10:A:GLN:H	10	0.8
(3,560)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.8
(1,623)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	10	0.8
(1,469)	1:7:A:LEU:HD11	1:10:A:GLN:H	7	0.8
(1,469)	1:7:A:LEU:HD12	1:10:A:GLN:H	7	0.8
(1,469)	1:7:A:LEU:HD13	1:10:A:GLN:H	7	0.8
(1,469)	1:7:A:LEU:HD11	1:10:A:GLN:H	10	0.8
(1,469)	1:7:A:LEU:HD12	1:10:A:GLN:H	10	0.8
(1,469)	1:7:A:LEU:HD13	1:10:A:GLN:H	10	0.8
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	9	0.79
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	9	0.79
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	9	0.79
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	9	0.79
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	9	0.79
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	9	0.79
(4,55)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	9	0.79
(3,575)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	1	0.79
(3,575)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	0.79
(3,575)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.79
(1,638)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	1	0.79
(1,638)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	0.79
(1,638)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.79
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	9	0.79
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	9	0.79
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	9	0.79
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	9	0.79
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	9	0.79
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	9	0.79
(1,559)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	9	0.79
(3,575)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	0.78
(3,575)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	0.78
(1,638)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	0.78
(1,638)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	0.78
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	6	0.77
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	6	0.77
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	6	0.77
(4,55)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	2	0.77
(4,16)	1:7:A:LEU:H	1:7:A:LEU:HB2	7	0.77
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	6	0.77
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	6	0.77
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	6	0.77
(1,559)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	2	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HB2	7	0.77
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	3	0.76
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	3	0.76
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	3	0.76
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	0.76
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	0.76
(4,56)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	0.76
(4,46)	1:7:A:LEU:HD11	1:10:A:GLN:H	1	0.76
(4,46)	1:7:A:LEU:HD12	1:10:A:GLN:H	1	0.76
(4,46)	1:7:A:LEU:HD13	1:10:A:GLN:H	1	0.76
(4,25)	1:24:A:PRO:HA	1:25:A:SER:H	6	0.76
(4,16)	1:7:A:LEU:H	1:7:A:LEU:HB2	5	0.76
(4,16)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.76
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	3	0.76
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	3	0.76
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	3	0.76
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB1	10	0.76
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB2	10	0.76
(1,563)	1:3:A:GLU:HB2	1:4:A:ALA:HB3	10	0.76
(1,469)	1:7:A:LEU:HD11	1:10:A:GLN:H	1	0.76
(1,469)	1:7:A:LEU:HD12	1:10:A:GLN:H	1	0.76
(1,469)	1:7:A:LEU:HD13	1:10:A:GLN:H	1	0.76
(1,285)	1:24:A:PRO:HA	1:25:A:SER:H	6	0.76
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HB2	5	0.76
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.76
(4,46)	1:7:A:LEU:HD11	1:10:A:GLN:H	2	0.75
(4,46)	1:7:A:LEU:HD12	1:10:A:GLN:H	2	0.75
(4,46)	1:7:A:LEU:HD13	1:10:A:GLN:H	2	0.75
(4,46)	1:7:A:LEU:HD11	1:10:A:GLN:H	5	0.75
(4,46)	1:7:A:LEU:HD12	1:10:A:GLN:H	5	0.75
(4,46)	1:7:A:LEU:HD13	1:10:A:GLN:H	5	0.75
(4,25)	1:24:A:PRO:HA	1:25:A:SER:H	9	0.75
(4,16)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.75
(3,575)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	0.75
(1,638)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	0.75
(1,469)	1:7:A:LEU:HD11	1:10:A:GLN:H	2	0.75
(1,469)	1:7:A:LEU:HD12	1:10:A:GLN:H	2	0.75
(1,469)	1:7:A:LEU:HD13	1:10:A:GLN:H	2	0.75
(1,469)	1:7:A:LEU:HD11	1:10:A:GLN:H	5	0.75
(1,469)	1:7:A:LEU:HD12	1:10:A:GLN:H	5	0.75
(1,469)	1:7:A:LEU:HD13	1:10:A:GLN:H	5	0.75
(1,285)	1:24:A:PRO:HA	1:25:A:SER:H	9	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.75
(4,16)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.74
(4,16)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.74
(3,560)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	2	0.74
(3,330)	1:21:A:ARG:HB3	1:21:A:ARG:HH11	7	0.74
(3,330)	1:21:A:ARG:HB3	1:21:A:ARG:HH12	7	0.74
(1,623)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	2	0.74
(1,361)	1:21:A:ARG:HB3	1:21:A:ARG:HH11	7	0.74
(1,361)	1:21:A:ARG:HB3	1:21:A:ARG:HH12	7	0.74
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.74
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.74
(4,25)	1:24:A:PRO:HA	1:25:A:SER:H	3	0.73
(4,25)	1:24:A:PRO:HA	1:25:A:SER:H	10	0.73
(4,16)	1:7:A:LEU:H	1:7:A:LEU:HB2	2	0.73
(4,16)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.73
(1,285)	1:24:A:PRO:HA	1:25:A:SER:H	3	0.73
(1,285)	1:24:A:PRO:HA	1:25:A:SER:H	10	0.73
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HB2	2	0.73
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.73
(4,16)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.72
(3,560)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	3	0.72
(1,623)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	3	0.72
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.72
(3,560)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	1	0.71
(1,623)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	1	0.71
(4,16)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.7
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.7
(4,46)	1:7:A:LEU:HD11	1:10:A:GLN:H	9	0.69
(4,46)	1:7:A:LEU:HD12	1:10:A:GLN:H	9	0.69
(4,46)	1:7:A:LEU:HD13	1:10:A:GLN:H	9	0.69
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD21	8	0.69
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD22	8	0.69
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD23	8	0.69
(3,560)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	5	0.69
(3,487)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	7	0.69
(1,623)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	5	0.69
(1,540)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	7	0.69
(1,469)	1:7:A:LEU:HD11	1:10:A:GLN:H	9	0.69
(1,469)	1:7:A:LEU:HD12	1:10:A:GLN:H	9	0.69
(1,469)	1:7:A:LEU:HD13	1:10:A:GLN:H	9	0.69
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD21	8	0.69
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD22	8	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD23	8	0.69
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD21	7	0.68
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD22	7	0.68
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD23	7	0.68
(3,487)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	0.68
(3,146)	1:14:A:ASP:H	1:14:A:ASP:HB3	2	0.68
(1,540)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	0.68
(1,483)	1:5:A:VAL:HB	1:6:A:ARG:H	10	0.68
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD21	7	0.68
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD22	7	0.68
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD23	7	0.68
(1,168)	1:14:A:ASP:H	1:14:A:ASP:HB3	2	0.68
(4,48)	1:5:A:VAL:HB	1:6:A:ARG:H	3	0.67
(4,48)	1:5:A:VAL:HB	1:6:A:ARG:H	10	0.67
(3,282)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	4	0.67
(3,282)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	4	0.67
(3,197)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	7	0.67
(3,146)	1:14:A:ASP:H	1:14:A:ASP:HB3	1	0.67
(3,146)	1:14:A:ASP:H	1:14:A:ASP:HB3	7	0.67
(3,146)	1:14:A:ASP:H	1:14:A:ASP:HB3	10	0.67
(1,483)	1:5:A:VAL:HB	1:6:A:ARG:H	3	0.67
(1,310)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	4	0.67
(1,310)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	4	0.67
(1,220)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	7	0.67
(1,168)	1:14:A:ASP:H	1:14:A:ASP:HB3	1	0.67
(1,168)	1:14:A:ASP:H	1:14:A:ASP:HB3	7	0.67
(1,168)	1:14:A:ASP:H	1:14:A:ASP:HB3	10	0.67
(3,282)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	3	0.66
(3,282)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	3	0.66
(1,310)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	3	0.66
(1,310)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	3	0.66
(4,64)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	9	0.65
(4,64)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	9	0.65
(4,64)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	9	0.65
(4,48)	1:5:A:VAL:HB	1:6:A:ARG:H	4	0.65
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD21	9	0.65
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD22	9	0.65
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD23	9	0.65
(4,24)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	4	0.65
(4,24)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.65
(3,560)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	4	0.65
(3,146)	1:14:A:ASP:H	1:14:A:ASP:HB3	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,146)	1:14:A:ASP:H	1:14:A:ASP:HB3	6	0.65
(3,146)	1:14:A:ASP:H	1:14:A:ASP:HB3	8	0.65
(3,146)	1:14:A:ASP:H	1:14:A:ASP:HB3	9	0.65
(1,648)	1:5:A:VAL:HG21	1:6:A:ARG:HG3	9	0.65
(1,648)	1:5:A:VAL:HG22	1:6:A:ARG:HG3	9	0.65
(1,648)	1:5:A:VAL:HG23	1:6:A:ARG:HG3	9	0.65
(1,623)	1:11:A:TRP:HZ2	1:23:A:PRO:HB2	4	0.65
(1,483)	1:5:A:VAL:HB	1:6:A:ARG:H	4	0.65
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD21	9	0.65
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD22	9	0.65
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD23	9	0.65
(1,248)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	4	0.65
(1,248)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	5	0.65
(1,168)	1:14:A:ASP:H	1:14:A:ASP:HB3	3	0.65
(1,168)	1:14:A:ASP:H	1:14:A:ASP:HB3	6	0.65
(1,168)	1:14:A:ASP:H	1:14:A:ASP:HB3	8	0.65
(1,168)	1:14:A:ASP:H	1:14:A:ASP:HB3	9	0.65
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD21	1	0.64
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD22	1	0.64
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD23	1	0.64
(4,24)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	10	0.64
(3,607)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	8	0.64
(3,607)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	8	0.64
(3,607)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	8	0.64
(3,282)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	2	0.64
(3,282)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	2	0.64
(3,197)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	8	0.64
(1,679)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	8	0.64
(1,679)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	8	0.64
(1,679)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	8	0.64
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD21	1	0.64
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD22	1	0.64
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD23	1	0.64
(1,310)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	2	0.64
(1,310)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	2	0.64
(1,248)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	10	0.64
(1,220)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	8	0.64
(4,66)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	2	0.63
(4,66)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	2	0.63
(4,66)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	2	0.63
(3,607)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	5	0.63
(3,607)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,607)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	5	0.63
(3,146)	1:14:A:ASP:H	1:14:A:ASP:HB3	4	0.63
(2,1)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	7	0.63
(2,1)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	7	0.63
(1,679)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	5	0.63
(1,679)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	5	0.63
(1,679)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	5	0.63
(1,653)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	2	0.63
(1,653)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	2	0.63
(1,653)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	2	0.63
(1,168)	1:14:A:ASP:H	1:14:A:ASP:HB3	4	0.63
(3,417)	1:8:A:TYR:H	1:24:A:PRO:HB3	4	0.62
(3,321)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	2	0.62
(3,282)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	1	0.62
(3,282)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	1	0.62
(3,282)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	0.62
(3,282)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	0.62
(1,459)	1:8:A:TYR:H	1:24:A:PRO:HB3	4	0.62
(1,352)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	2	0.62
(1,310)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	1	0.62
(1,310)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	1	0.62
(1,310)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	9	0.62
(1,310)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	9	0.62
(3,607)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	1	0.61
(3,607)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	1	0.61
(3,607)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	1	0.61
(3,282)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.61
(3,282)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.61
(1,679)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	1	0.61
(1,679)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	1	0.61
(1,679)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	1	0.61
(1,310)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	10	0.61
(1,310)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	10	0.61
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	7	0.6
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	7	0.6
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	7	0.6
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	9	0.6
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	9	0.6
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	9	0.6
(4,7)	1:6:A:ARG:H	1:6:A:ARG:HB2	9	0.6
(4,7)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.6
(3,607)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	2	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,607)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	2	0.6
(3,607)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	2	0.6
(3,607)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	7	0.6
(3,607)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	7	0.6
(3,607)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	7	0.6
(3,487)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	0.6
(3,487)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	0.6
(3,487)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.6
(3,487)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.6
(3,321)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	4	0.6
(3,205)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.6
(3,205)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.6
(3,205)	1:21:A:ARG:H	1:21:A:ARG:HB3	8	0.6
(3,205)	1:21:A:ARG:H	1:21:A:ARG:HB3	9	0.6
(3,205)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.6
(1,679)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	2	0.6
(1,679)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	2	0.6
(1,679)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	2	0.6
(1,679)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	7	0.6
(1,679)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	7	0.6
(1,679)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	7	0.6
(1,540)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	0.6
(1,540)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	0.6
(1,540)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.6
(1,540)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	10	0.6
(1,352)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	4	0.6
(1,228)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.6
(1,228)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.6
(1,228)	1:21:A:ARG:H	1:21:A:ARG:HB3	8	0.6
(1,228)	1:21:A:ARG:H	1:21:A:ARG:HB3	9	0.6
(1,228)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.6
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD11	7	0.6
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD12	7	0.6
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD13	7	0.6
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD11	9	0.6
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD12	9	0.6
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD13	9	0.6
(1,49)	1:6:A:ARG:H	1:6:A:ARG:HB2	9	0.6
(1,49)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.6
(4,7)	1:6:A:ARG:H	1:6:A:ARG:HB2	4	0.59
(3,487)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	0.59
(3,487)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,282)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	6	0.59
(3,282)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	6	0.59
(3,205)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.59
(3,205)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.59
(1,540)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	0.59
(1,540)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	6	0.59
(1,310)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	6	0.59
(1,310)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	6	0.59
(1,228)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.59
(1,228)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.59
(1,49)	1:6:A:ARG:H	1:6:A:ARG:HB2	4	0.59
(4,55)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	4	0.58
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	6	0.58
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	6	0.58
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	6	0.58
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	4	0.58
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	4	0.58
(3,487)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	0.58
(3,487)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	0.58
(3,392)	1:9:A:ILE:H	1:10:A:GLN:HB3	2	0.58
(3,282)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	5	0.58
(3,282)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	5	0.58
(3,205)	1:21:A:ARG:H	1:21:A:ARG:HB3	4	0.58
(1,559)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	4	0.58
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	4	0.58
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	4	0.58
(1,540)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	0.58
(1,540)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	0.58
(1,431)	1:9:A:ILE:H	1:10:A:GLN:HB3	2	0.58
(1,352)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	5	0.58
(1,310)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	5	0.58
(1,310)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	5	0.58
(1,228)	1:21:A:ARG:H	1:21:A:ARG:HB3	4	0.58
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD11	6	0.58
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD12	6	0.58
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD13	6	0.58
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	1	0.57
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	1	0.57
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	5	0.57
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	5	0.57
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	6	0.57
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	6	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,321)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	1	0.57
(3,321)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	5	0.57
(3,282)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	8	0.57
(3,282)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	8	0.57
(3,205)	1:21:A:ARG:H	1:21:A:ARG:HB3	1	0.57
(3,205)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.57
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	1	0.57
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	1	0.57
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	5	0.57
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	5	0.57
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	6	0.57
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	6	0.57
(1,352)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	1	0.57
(1,310)	1:8:A:TYR:HE1	1:24:A:PRO:HD3	8	0.57
(1,310)	1:8:A:TYR:HE2	1:24:A:PRO:HD3	8	0.57
(1,228)	1:21:A:ARG:H	1:21:A:ARG:HB3	1	0.57
(1,228)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.57
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	3	0.56
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	3	0.56
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	10	0.56
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	10	0.56
(3,321)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	3	0.56
(3,321)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	9	0.56
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	3	0.56
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	3	0.56
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	10	0.56
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	10	0.56
(1,352)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	3	0.56
(1,352)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	9	0.56
(4,66)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	9	0.55
(4,66)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	9	0.55
(4,66)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	9	0.55
(4,21)	1:10:A:GLN:H	1:10:A:GLN:HG3	9	0.55
(1,653)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	9	0.55
(1,653)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	9	0.55
(1,653)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	9	0.55
(1,125)	1:10:A:GLN:H	1:10:A:GLN:HG3	9	0.55
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	2	0.54
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	2	0.54
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	2	0.54
(4,7)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	0.54
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	7	0.54
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	9	0.54
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	9	0.54
(3,321)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	6	0.54
(2,1)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	2	0.54
(2,1)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	2	0.54
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	7	0.54
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	7	0.54
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	9	0.54
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	9	0.54
(1,352)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	6	0.54
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD11	2	0.54
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD12	2	0.54
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD13	2	0.54
(1,49)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	0.54
(4,55)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	7	0.53
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD21	2	0.53
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD22	2	0.53
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD23	2	0.53
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	3	0.53
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	3	0.53
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	3	0.53
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	4	0.53
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	4	0.53
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	4	0.53
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.53
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.53
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.53
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	5	0.53
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	5	0.53
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	5	0.53
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	8	0.53
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	8	0.53
(3,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	4	0.53
(1,559)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	7	0.53
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	8	0.53
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	8	0.53
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD21	2	0.53
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD22	2	0.53
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD23	2	0.53
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	4	0.53
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	3	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	3	0.53
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	3	0.53
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	4	0.53
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	4	0.53
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	4	0.53
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	10	0.53
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	10	0.53
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	10	0.53
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD11	5	0.53
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD12	5	0.53
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD13	5	0.53
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	1	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	1	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	1	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	5	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	5	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	5	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	6	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	6	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	6	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	8	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	8	0.52
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	8	0.52
(3,458)	1:23:A:PRO:HB3	1:25:A:SER:H	6	0.52
(3,321)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	10	0.52
(3,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	1	0.52
(3,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	3	0.52
(3,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	5	0.52
(3,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	6	0.52
(3,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	7	0.52
(2,1)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	5	0.52
(2,1)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	5	0.52
(2,1)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	8	0.52
(2,1)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	8	0.52
(1,508)	1:23:A:PRO:HB3	1:25:A:SER:H	6	0.52
(1,352)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	10	0.52
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	1	0.52
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	3	0.52
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	5	0.52
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	6	0.52
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	7	0.52
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	8	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	1	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	1	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	1	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	5	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	5	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	5	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	6	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	6	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	6	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	8	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	8	0.52
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	8	0.52
(4,55)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	1	0.51
(4,55)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	8	0.51
(4,43)	1:7:A:LEU:HB2	1:8:A:TYR:H	2	0.51
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	7	0.51
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	7	0.51
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	7	0.51
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	1	0.51
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	1	0.51
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	1	0.51
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	8	0.51
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	8	0.51
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	8	0.51
(3,607)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	4	0.51
(3,607)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	4	0.51
(3,607)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	4	0.51
(3,460)	1:24:A:PRO:HB3	1:25:A:SER:H	7	0.51
(3,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	8	0.51
(3,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	9	0.51
(2,1)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	1	0.51
(2,1)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	1	0.51
(1,679)	1:7:A:LEU:HD21	1:24:A:PRO:HB3	4	0.51
(1,679)	1:7:A:LEU:HD22	1:24:A:PRO:HB3	4	0.51
(1,679)	1:7:A:LEU:HD23	1:24:A:PRO:HB3	4	0.51
(1,559)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	1	0.51
(1,559)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	8	0.51
(1,510)	1:24:A:PRO:HB3	1:25:A:SER:H	7	0.51
(1,460)	1:7:A:LEU:HB2	1:8:A:TYR:H	2	0.51
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	9	0.51
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	7	0.51
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	7	0.51
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD11	1	0.51
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD12	1	0.51
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD13	1	0.51
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD11	8	0.51
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD12	8	0.51
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD13	8	0.51
(4,41)	1:12:A:LEU:HA	1:13:A:LYS:H	3	0.5
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.5
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.5
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	2	0.5
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	2	0.5
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	2	0.5
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	9	0.5
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	9	0.5
(4,13)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	9	0.5
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	10	0.5
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	10	0.5
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	10	0.5
(4,7)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.5
(4,7)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.5
(4,7)	1:6:A:ARG:H	1:6:A:ARG:HB2	8	0.5
(4,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	2	0.5
(3,412)	1:18:A:SER:HB2	1:19:A:SER:H	8	0.5
(1,454)	1:18:A:SER:HB2	1:19:A:SER:H	8	0.5
(1,440)	1:12:A:LEU:HA	1:13:A:LYS:H	3	0.5
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.5
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.5
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	2	0.5
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	2	0.5
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	2	0.5
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	9	0.5
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	9	0.5
(1,72)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	9	0.5
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD11	10	0.5
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD12	10	0.5
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD13	10	0.5
(1,49)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.5
(1,49)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.5
(1,49)	1:6:A:ARG:H	1:6:A:ARG:HB2	8	0.5
(1,35)	1:6:A:ARG:HA	1:6:A:ARG:HG2	2	0.5
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD21	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD22	5	0.49
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD23	5	0.49
(4,41)	1:12:A:LEU:HA	1:13:A:LYS:H	10	0.49
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.49
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.49
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.49
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.49
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.49
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.49
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.49
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.49
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	4	0.49
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	4	0.49
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	4	0.49
(4,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	1	0.49
(3,458)	1:23:A:PRO:HB3	1:25:A:SER:H	9	0.49
(3,412)	1:18:A:SER:HB2	1:19:A:SER:H	6	0.49
(1,508)	1:23:A:PRO:HB3	1:25:A:SER:H	9	0.49
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD21	5	0.49
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD22	5	0.49
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD23	5	0.49
(1,454)	1:18:A:SER:HB2	1:19:A:SER:H	6	0.49
(1,440)	1:12:A:LEU:HA	1:13:A:LYS:H	10	0.49
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.49
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.49
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.49
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.49
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.49
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.49
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.49
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.49
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD11	4	0.49
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD12	4	0.49
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD13	4	0.49
(1,35)	1:6:A:ARG:HA	1:6:A:ARG:HG2	1	0.49
(4,55)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	6	0.48
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD21	3	0.48
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD22	3	0.48
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD23	3	0.48
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.48
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.48
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.48
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.48
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.48
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.48
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.48
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG2	6	0.48
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG3	6	0.48
(3,460)	1:24:A:PRO:HB3	1:25:A:SER:H	4	0.48
(3,460)	1:24:A:PRO:HB3	1:25:A:SER:H	5	0.48
(3,429)	1:11:A:TRP:H	1:24:A:PRO:HG2	4	0.48
(3,392)	1:9:A:ILE:H	1:10:A:GLN:HB3	9	0.48
(1,559)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	6	0.48
(1,510)	1:24:A:PRO:HB3	1:25:A:SER:H	4	0.48
(1,510)	1:24:A:PRO:HB3	1:25:A:SER:H	5	0.48
(1,476)	1:11:A:TRP:H	1:24:A:PRO:HG2	4	0.48
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD21	3	0.48
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD22	3	0.48
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD23	3	0.48
(1,431)	1:9:A:ILE:H	1:10:A:GLN:HB3	9	0.48
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.48
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.48
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.48
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.48
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.48
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.48
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.48
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.48
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG2	6	0.48
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG3	6	0.48
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	8	0.47
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	8	0.47
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	8	0.47
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	8	0.47
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	8	0.47
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	8	0.47
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	8	0.47
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	8	0.47
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	8	0.47
(4,41)	1:12:A:LEU:HA	1:13:A:LYS:H	1	0.47
(4,41)	1:12:A:LEU:HA	1:13:A:LYS:H	4	0.47
(4,41)	1:12:A:LEU:HA	1:13:A:LYS:H	5	0.47
(4,41)	1:12:A:LEU:HA	1:13:A:LYS:H	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,41)	1:12:A:LEU:HA	1:13:A:LYS:H	8	0.47
(3,499)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	4	0.47
(3,100)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	9	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	2	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	2	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	2	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	7	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	7	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	7	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.47
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.47
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	8	0.47
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	8	0.47
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	8	0.47
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	8	0.47
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	8	0.47
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	8	0.47
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	8	0.47
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	8	0.47
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	8	0.47
(1,553)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	4	0.47
(1,440)	1:12:A:LEU:HA	1:13:A:LYS:H	1	0.47
(1,440)	1:12:A:LEU:HA	1:13:A:LYS:H	4	0.47
(1,440)	1:12:A:LEU:HA	1:13:A:LYS:H	5	0.47
(1,440)	1:12:A:LEU:HA	1:13:A:LYS:H	7	0.47
(1,440)	1:12:A:LEU:HA	1:13:A:LYS:H	8	0.47
(1,119)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	9	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	2	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	2	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	2	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	5	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	5	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	5	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	7	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	7	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	7	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	8	0.47
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	8	0.47
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	9	0.46
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	9	0.46
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	9	0.46
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	9	0.46
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	9	0.46
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	9	0.46
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	9	0.46
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	9	0.46
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	9	0.46
(4,43)	1:7:A:LEU:HB2	1:8:A:TYR:H	7	0.46
(4,41)	1:12:A:LEU:HA	1:13:A:LYS:H	6	0.46
(4,33)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.46
(4,7)	1:6:A:ARG:H	1:6:A:ARG:HB2	2	0.46
(3,606)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	2	0.46
(3,606)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	2	0.46
(3,606)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	2	0.46
(3,460)	1:24:A:PRO:HB3	1:25:A:SER:H	1	0.46
(3,303)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	1	0.46
(3,303)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	2	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	9	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	9	0.46
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	9	0.46
(1,678)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	2	0.46
(1,678)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	2	0.46
(1,678)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	2	0.46
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	9	0.46
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	9	0.46
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	9	0.46
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	9	0.46
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	9	0.46
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	9	0.46
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	9	0.46
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	9	0.46
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	9	0.46
(1,510)	1:24:A:PRO:HB3	1:25:A:SER:H	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,460)	1:7:A:LEU:HB2	1:8:A:TYR:H	7	0.46
(1,440)	1:12:A:LEU:HA	1:13:A:LYS:H	6	0.46
(1,381)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	4	0.46
(1,332)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	1	0.46
(1,332)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	2	0.46
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	1	0.46
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	1	0.46
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	1	0.46
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	6	0.46
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	6	0.46
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	6	0.46
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	9	0.46
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	9	0.46
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	9	0.46
(1,49)	1:6:A:ARG:H	1:6:A:ARG:HB2	2	0.46
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	1	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	1	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	1	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	1	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	1	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	1	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	1	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	1	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	1	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	2	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	2	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	2	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	2	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	2	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	2	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	2	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	2	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	2	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	5	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	5	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	5	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	5	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	5	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	5	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	5	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	5	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	6	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	6	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	6	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	6	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	6	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	6	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	6	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	6	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	6	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	7	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	7	0.45
(4,61)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	7	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	7	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	7	0.45
(4,61)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	7	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	7	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	7	0.45
(4,61)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	7	0.45
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	10	0.45
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	10	0.45
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	10	0.45
(4,55)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	5	0.45
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD21	6	0.45
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD22	6	0.45
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD23	6	0.45
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD21	10	0.45
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD22	10	0.45
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD23	10	0.45
(4,43)	1:7:A:LEU:HB2	1:8:A:TYR:H	8	0.45
(4,43)	1:7:A:LEU:HB2	1:8:A:TYR:H	9	0.45
(4,41)	1:12:A:LEU:HA	1:13:A:LYS:H	9	0.45
(4,36)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	1	0.45
(4,36)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	2	0.45
(4,36)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	4	0.45
(4,36)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	5	0.45
(4,36)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	9	0.45
(4,21)	1:10:A:GLN:H	1:10:A:GLN:HG3	1	0.45
(4,21)	1:10:A:GLN:H	1:10:A:GLN:HG3	5	0.45
(4,21)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.45
(4,21)	1:10:A:GLN:H	1:10:A:GLN:HG3	7	0.45
(3,606)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	1	0.45
(3,606)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,606)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	1	0.45
(3,606)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	8	0.45
(3,606)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	8	0.45
(3,606)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	8	0.45
(3,460)	1:24:A:PRO:HB3	1:25:A:SER:H	2	0.45
(3,460)	1:24:A:PRO:HB3	1:25:A:SER:H	8	0.45
(3,321)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	7	0.45
(3,303)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	5	0.45
(3,303)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	6	0.45
(3,198)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	7	0.45
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.45
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.45
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.45
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.45
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.45
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.45
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.45
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.45
(3,69)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.45
(1,678)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	1	0.45
(1,678)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	1	0.45
(1,678)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	1	0.45
(1,678)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	8	0.45
(1,678)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	8	0.45
(1,678)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	8	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	1	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	1	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	1	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	1	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	1	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	1	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	1	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	1	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	1	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	2	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	2	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	2	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	2	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	2	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	2	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	2	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	2	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	5	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	5	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	5	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	5	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	5	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	5	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	5	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	5	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	5	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	6	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	6	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	6	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	6	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	6	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	6	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	6	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	6	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	6	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	7	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	7	0.45
(1,603)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	7	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	7	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	7	0.45
(1,603)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	7	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	7	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	7	0.45
(1,603)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	7	0.45
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	10	0.45
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	10	0.45
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	10	0.45
(1,559)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	5	0.45
(1,510)	1:24:A:PRO:HB3	1:25:A:SER:H	2	0.45
(1,510)	1:24:A:PRO:HB3	1:25:A:SER:H	8	0.45
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD21	6	0.45
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD22	6	0.45
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD23	6	0.45
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD21	10	0.45
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD22	10	0.45
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD23	10	0.45
(1,460)	1:7:A:LEU:HB2	1:8:A:TYR:H	8	0.45
(1,460)	1:7:A:LEU:HB2	1:8:A:TYR:H	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:12:A:LEU:HA	1:13:A:LYS:H	9	0.45
(1,397)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	1	0.45
(1,397)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	2	0.45
(1,397)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	4	0.45
(1,397)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	5	0.45
(1,397)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	9	0.45
(1,352)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	7	0.45
(1,332)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	5	0.45
(1,332)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	6	0.45
(1,221)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	7	0.45
(1,125)	1:10:A:GLN:H	1:10:A:GLN:HG3	1	0.45
(1,125)	1:10:A:GLN:H	1:10:A:GLN:HG3	5	0.45
(1,125)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.45
(1,125)	1:10:A:GLN:H	1:10:A:GLN:HG3	7	0.45
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	3	0.45
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	3	0.45
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	3	0.45
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	4	0.45
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	4	0.45
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	4	0.45
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD11	10	0.45
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD12	10	0.45
(1,84)	1:7:A:LEU:HB3	1:7:A:LEU:HD13	10	0.45
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	1	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	1	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	1	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	4	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	4	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	4	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	6	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	6	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	6	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	9	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	9	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	9	0.44
(4,55)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	3	0.44
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD21	4	0.44
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD22	4	0.44
(4,45)	1:11:A:TRP:H	1:12:A:LEU:HD23	4	0.44
(4,43)	1:7:A:LEU:HB2	1:8:A:TYR:H	5	0.44
(4,41)	1:12:A:LEU:HA	1:13:A:LYS:H	2	0.44
(4,36)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,36)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	6	0.44
(4,36)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	7	0.44
(4,36)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	8	0.44
(4,36)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.44
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.44
(4,28)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.44
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG2	8	0.44
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG3	8	0.44
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG2	9	0.44
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG3	9	0.44
(3,321)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	8	0.44
(3,303)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	4	0.44
(3,198)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	8	0.44
(3,100)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	3	0.44
(3,100)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	4	0.44
(3,100)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	5	0.44
(3,100)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	6	0.44
(3,100)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	7	0.44
(3,100)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	8	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	1	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	1	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	1	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	4	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	4	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	4	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	6	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	6	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	6	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	9	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	9	0.44
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	9	0.44
(1,559)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	3	0.44
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD21	4	0.44
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD22	4	0.44
(1,464)	1:11:A:TRP:H	1:12:A:LEU:HD23	4	0.44
(1,460)	1:7:A:LEU:HB2	1:8:A:TYR:H	5	0.44
(1,440)	1:12:A:LEU:HA	1:13:A:LYS:H	2	0.44
(1,397)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	3	0.44
(1,397)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	6	0.44
(1,397)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	7	0.44
(1,397)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	8	0.44
(1,397)	1:11:A:TRP:HE3	1:11:A:TRP:HH2	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:11:A:TRP:HH2	1:17:A:PRO:HB2	8	0.44
(1,332)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	4	0.44
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.44
(1,307)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.44
(1,221)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	8	0.44
(1,119)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	3	0.44
(1,119)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	4	0.44
(1,119)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	5	0.44
(1,119)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	6	0.44
(1,119)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	7	0.44
(1,119)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	8	0.44
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG2	8	0.44
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG3	8	0.44
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG2	9	0.44
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG3	9	0.44
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	7	0.43
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	7	0.43
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	7	0.43
(4,43)	1:7:A:LEU:HB2	1:8:A:TYR:H	1	0.43
(4,21)	1:10:A:GLN:H	1:10:A:GLN:HG3	4	0.43
(4,21)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.43
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG11	3	0.43
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG12	3	0.43
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG13	3	0.43
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG11	4	0.43
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG12	4	0.43
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG13	4	0.43
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG2	5	0.43
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG3	5	0.43
(3,489)	1:11:A:TRP:HB2	1:24:A:PRO:HD2	7	0.43
(3,100)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	1	0.43
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	7	0.43
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	7	0.43
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	7	0.43
(1,543)	1:11:A:TRP:HB2	1:24:A:PRO:HD2	7	0.43
(1,460)	1:7:A:LEU:HB2	1:8:A:TYR:H	1	0.43
(1,125)	1:10:A:GLN:H	1:10:A:GLN:HG3	4	0.43
(1,125)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.43
(1,119)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	1	0.43
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG11	3	0.43
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG12	3	0.43
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG13	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG11	4	0.43
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG12	4	0.43
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG13	4	0.43
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG2	5	0.43
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG3	5	0.43
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	8	0.42
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	8	0.42
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	8	0.42
(4,25)	1:24:A:PRO:HA	1:25:A:SER:H	8	0.42
(4,21)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.42
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.42
(4,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	9	0.42
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG11	10	0.42
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG12	10	0.42
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG13	10	0.42
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG2	2	0.42
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG3	2	0.42
(3,343)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	7	0.42
(3,303)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	3	0.42
(3,146)	1:14:A:ASP:H	1:14:A:ASP:HB3	5	0.42
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	8	0.42
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	8	0.42
(1,374)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	7	0.42
(1,332)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	3	0.42
(1,332)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	10	0.42
(1,285)	1:24:A:PRO:HA	1:25:A:SER:H	8	0.42
(1,168)	1:14:A:ASP:H	1:14:A:ASP:HB3	5	0.42
(1,125)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.42
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.42
(1,35)	1:6:A:ARG:HA	1:6:A:ARG:HG2	9	0.42
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG11	10	0.42
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG12	10	0.42
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG13	10	0.42
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG2	2	0.42
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG3	2	0.42
(4,67)	1:8:A:TYR:HA	1:9:A:ILE:H	1	0.41
(4,67)	1:8:A:TYR:HA	1:9:A:ILE:H	2	0.41
(4,67)	1:8:A:TYR:HA	1:9:A:ILE:H	3	0.41
(4,67)	1:8:A:TYR:HA	1:9:A:ILE:H	8	0.41
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	2	0.41
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	2	0.41
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	2	0.41
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	5	0.41
(4,60)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	5	0.41
(4,55)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	10	0.41
(4,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.41
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.41
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.41
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.41
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.41
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.41
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.41
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.41
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.41
(4,11)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.41
(4,3)	1:3:A:GLU:H	1:3:A:GLU:HB3	1	0.41
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG2	7	0.41
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG3	7	0.41
(3,606)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	5	0.41
(3,606)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	5	0.41
(3,606)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	5	0.41
(3,485)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	6	0.41
(3,485)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	6	0.41
(3,458)	1:23:A:PRO:HB3	1:25:A:SER:H	10	0.41
(3,343)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	1	0.41
(3,303)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	10	0.41
(1,678)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	5	0.41
(1,678)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	5	0.41
(1,678)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	5	0.41
(1,656)	1:8:A:TYR:HA	1:9:A:ILE:H	1	0.41
(1,656)	1:8:A:TYR:HA	1:9:A:ILE:H	2	0.41
(1,656)	1:8:A:TYR:HA	1:9:A:ILE:H	3	0.41
(1,656)	1:8:A:TYR:HA	1:9:A:ILE:H	8	0.41
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	2	0.41
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	2	0.41
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	2	0.41
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD21	5	0.41
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD22	5	0.41
(1,599)	1:9:A:ILE:HG12	1:12:A:LEU:HD23	5	0.41
(1,559)	1:7:A:LEU:HB2	1:10:A:GLN:HB3	10	0.41
(1,538)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	6	0.41
(1,538)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	6	0.41
(1,508)	1:23:A:PRO:HB3	1:25:A:SER:H	10	0.41
(1,374)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	3	0.41
(1,124)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.41
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.41
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.41
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.41
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.41
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.41
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.41
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.41
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.41
(1,70)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.41
(1,14)	1:3:A:GLU:H	1:3:A:GLU:HB3	1	0.41
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG2	7	0.41
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG3	7	0.41
(4,67)	1:8:A:TYR:HA	1:9:A:ILE:H	4	0.4
(4,67)	1:8:A:TYR:HA	1:9:A:ILE:H	5	0.4
(4,67)	1:8:A:TYR:HA	1:9:A:ILE:H	7	0.4
(4,43)	1:7:A:LEU:HB2	1:8:A:TYR:H	4	0.4
(4,43)	1:7:A:LEU:HB2	1:8:A:TYR:H	6	0.4
(4,33)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.4
(4,33)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.4
(4,33)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.4
(4,30)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	0.4
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD11	3	0.4
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD12	3	0.4
(4,12)	1:9:A:ILE:H	1:9:A:ILE:HD13	3	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG11	1	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG12	1	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG13	1	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG11	2	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG12	2	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG13	2	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG11	5	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG12	5	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG13	5	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG11	6	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG12	6	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG13	6	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG11	7	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG12	7	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG13	7	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG11	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG12	8	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG13	8	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG11	9	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG12	9	0.4
(4,4)	1:5:A:VAL:HA	1:5:A:VAL:HG13	9	0.4
(4,1)	1:2:A:GLU:HA	1:3:A:GLU:H	7	0.4
(3,528)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	7	0.4
(3,528)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	7	0.4
(3,528)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	7	0.4
(3,485)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	1	0.4
(3,485)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	1	0.4
(3,384)	1:8:A:TYR:HB2	1:9:A:ILE:H	8	0.4
(3,343)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	3	0.4
(3,343)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	6	0.4
(3,343)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	8	0.4
(3,33)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	10	0.4
(1,656)	1:8:A:TYR:HA	1:9:A:ILE:H	4	0.4
(1,656)	1:8:A:TYR:HA	1:9:A:ILE:H	5	0.4
(1,656)	1:8:A:TYR:HA	1:9:A:ILE:H	7	0.4
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	4	0.4
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	4	0.4
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	4	0.4
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	4	0.4
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	4	0.4
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	4	0.4
(1,585)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	7	0.4
(1,585)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	7	0.4
(1,585)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	7	0.4
(1,538)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	1	0.4
(1,538)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	1	0.4
(1,460)	1:7:A:LEU:HB2	1:8:A:TYR:H	4	0.4
(1,460)	1:7:A:LEU:HB2	1:8:A:TYR:H	6	0.4
(1,422)	1:8:A:TYR:HB2	1:9:A:ILE:H	8	0.4
(1,381)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	2	0.4
(1,381)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	3	0.4
(1,381)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	5	0.4
(1,374)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	6	0.4
(1,374)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	8	0.4
(1,346)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	0.4
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD11	3	0.4
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD12	3	0.4
(1,71)	1:9:A:ILE:H	1:9:A:ILE:HD13	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	10	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG11	1	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG12	1	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG13	1	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG11	2	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG12	2	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG13	2	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG11	5	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG12	5	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG13	5	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG11	6	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG12	6	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG13	6	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG11	7	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG12	7	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG13	7	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG11	8	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG12	8	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG13	8	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG11	9	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG12	9	0.4
(1,22)	1:5:A:VAL:HA	1:5:A:VAL:HG13	9	0.4
(1,1)	1:2:A:GLU:HA	1:3:A:GLU:H	7	0.4
(4,67)	1:8:A:TYR:HA	1:9:A:ILE:H	9	0.39
(4,67)	1:8:A:TYR:HA	1:9:A:ILE:H	10	0.39
(4,62)	1:5:A:VAL:HG11	1:9:A:ILE:H	9	0.39
(4,62)	1:5:A:VAL:HG12	1:9:A:ILE:H	9	0.39
(4,62)	1:5:A:VAL:HG13	1:9:A:ILE:H	9	0.39
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	3	0.39
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	3	0.39
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	3	0.39
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	3	0.39
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	3	0.39
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	3	0.39
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	4	0.39
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	4	0.39
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	4	0.39
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	4	0.39
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	4	0.39
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	4	0.39
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	6	0.39
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	6	0.39
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	6	0.39
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	6	0.39
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	6	0.39
(4,42)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.39
(4,42)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.39
(4,42)	1:12:A:LEU:H	1:12:A:LEU:HB3	8	0.39
(4,42)	1:12:A:LEU:H	1:12:A:LEU:HB3	9	0.39
(4,39)	1:1:A:GLU:HG2	1:4:A:ALA:H	9	0.39
(4,39)	1:1:A:GLU:HG3	1:4:A:ALA:H	9	0.39
(4,33)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.39
(4,33)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.39
(4,33)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.39
(4,30)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	0.39
(4,1)	1:2:A:GLU:HA	1:3:A:GLU:H	1	0.39
(4,1)	1:2:A:GLU:HA	1:3:A:GLU:H	9	0.39
(3,485)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	2	0.39
(3,485)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	2	0.39
(3,384)	1:8:A:TYR:HB2	1:9:A:ILE:H	5	0.39
(3,384)	1:8:A:TYR:HB2	1:9:A:ILE:H	7	0.39
(3,319)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	1	0.39
(3,319)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	3	0.39
(3,303)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	9	0.39
(3,100)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	2	0.39
(1,656)	1:8:A:TYR:HA	1:9:A:ILE:H	9	0.39
(1,656)	1:8:A:TYR:HA	1:9:A:ILE:H	10	0.39
(1,613)	1:5:A:VAL:HG11	1:9:A:ILE:H	9	0.39
(1,613)	1:5:A:VAL:HG12	1:9:A:ILE:H	9	0.39
(1,613)	1:5:A:VAL:HG13	1:9:A:ILE:H	9	0.39
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	3	0.39
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	3	0.39
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	3	0.39
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	3	0.39
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	3	0.39
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	3	0.39
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	6	0.39
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	6	0.39
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	6	0.39
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	6	0.39
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	6	0.39
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	6	0.39
(1,585)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	9	0.39
(1,585)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	9	0.39
(1,538)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	2	0.39
(1,538)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	2	0.39
(1,445)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.39
(1,445)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.39
(1,445)	1:12:A:LEU:H	1:12:A:LEU:HB3	8	0.39
(1,445)	1:12:A:LEU:H	1:12:A:LEU:HB3	9	0.39
(1,424)	1:1:A:GLU:HG2	1:4:A:ALA:H	9	0.39
(1,424)	1:1:A:GLU:HG3	1:4:A:ALA:H	9	0.39
(1,422)	1:8:A:TYR:HB2	1:9:A:ILE:H	5	0.39
(1,422)	1:8:A:TYR:HB2	1:9:A:ILE:H	7	0.39
(1,381)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	1	0.39
(1,381)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	6	0.39
(1,381)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	10	0.39
(1,350)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	1	0.39
(1,350)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	3	0.39
(1,346)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	0.39
(1,332)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	9	0.39
(1,119)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	2	0.39
(1,1)	1:2:A:GLU:HA	1:3:A:GLU:H	1	0.39
(1,1)	1:2:A:GLU:HA	1:3:A:GLU:H	9	0.39
(4,67)	1:8:A:TYR:HA	1:9:A:ILE:H	6	0.38
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD2	6	0.38
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD3	6	0.38
(4,42)	1:12:A:LEU:H	1:12:A:LEU:HB3	1	0.38
(4,42)	1:12:A:LEU:H	1:12:A:LEU:HB3	5	0.38
(4,42)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.38
(4,42)	1:12:A:LEU:H	1:12:A:LEU:HB3	7	0.38
(4,42)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.38
(4,33)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.38
(4,33)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.38
(4,33)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.38
(4,25)	1:24:A:PRO:HA	1:25:A:SER:H	2	0.38
(4,1)	1:2:A:GLU:HA	1:3:A:GLU:H	2	0.38
(4,1)	1:2:A:GLU:HA	1:3:A:GLU:H	8	0.38
(3,568)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	10	0.38
(3,528)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	5	0.38
(3,528)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	5	0.38
(3,528)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	5	0.38
(3,528)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	9	0.38
(3,528)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,528)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	9	0.38
(3,485)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	3	0.38
(3,485)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	3	0.38
(3,343)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	4	0.38
(3,343)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	9	0.38
(3,319)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	5	0.38
(3,319)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	6	0.38
(3,319)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	9	0.38
(3,319)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	10	0.38
(1,656)	1:8:A:TYR:HA	1:9:A:ILE:H	6	0.38
(1,631)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	10	0.38
(1,585)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	5	0.38
(1,585)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	5	0.38
(1,585)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	5	0.38
(1,538)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	3	0.38
(1,538)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	3	0.38
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD2	6	0.38
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD3	6	0.38
(1,445)	1:12:A:LEU:H	1:12:A:LEU:HB3	1	0.38
(1,445)	1:12:A:LEU:H	1:12:A:LEU:HB3	5	0.38
(1,445)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.38
(1,445)	1:12:A:LEU:H	1:12:A:LEU:HB3	7	0.38
(1,445)	1:12:A:LEU:H	1:12:A:LEU:HB3	10	0.38
(1,381)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	7	0.38
(1,381)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	8	0.38
(1,381)	1:11:A:TRP:HB2	1:11:A:TRP:HE3	9	0.38
(1,374)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	4	0.38
(1,374)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	9	0.38
(1,350)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	5	0.38
(1,350)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	6	0.38
(1,350)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	9	0.38
(1,350)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	10	0.38
(1,285)	1:24:A:PRO:HA	1:25:A:SER:H	2	0.38
(1,1)	1:2:A:GLU:HA	1:3:A:GLU:H	2	0.38
(1,1)	1:2:A:GLU:HA	1:3:A:GLU:H	8	0.38
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD21	10	0.37
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD22	10	0.37
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD23	10	0.37
(4,52)	1:1:A:GLU:HB2	1:2:A:GLU:HA	6	0.37
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD2	1	0.37
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD3	1	0.37
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD2	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD3	2	0.37
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD2	9	0.37
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD3	9	0.37
(4,42)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.37
(4,39)	1:1:A:GLU:HG2	1:4:A:ALA:H	1	0.37
(4,39)	1:1:A:GLU:HG3	1:4:A:ALA:H	1	0.37
(4,39)	1:1:A:GLU:HG2	1:4:A:ALA:H	2	0.37
(4,39)	1:1:A:GLU:HG3	1:4:A:ALA:H	2	0.37
(4,30)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	0.37
(4,30)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	0.37
(4,30)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.37
(4,7)	1:6:A:ARG:H	1:6:A:ARG:HB2	6	0.37
(4,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	3	0.37
(4,3)	1:3:A:GLU:H	1:3:A:GLU:HB3	2	0.37
(4,3)	1:3:A:GLU:H	1:3:A:GLU:HB3	7	0.37
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG2	1	0.37
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG3	1	0.37
(3,568)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	1	0.37
(3,528)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	8	0.37
(3,528)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	8	0.37
(3,528)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	8	0.37
(3,384)	1:8:A:TYR:HB2	1:9:A:ILE:H	3	0.37
(3,343)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	10	0.37
(3,319)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	4	0.37
(3,319)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	7	0.37
(3,319)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	8	0.37
(3,115)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	9	0.37
(1,631)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	1	0.37
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD21	10	0.37
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD22	10	0.37
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD23	10	0.37
(1,585)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	8	0.37
(1,585)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	8	0.37
(1,585)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	8	0.37
(1,529)	1:1:A:GLU:HB2	1:2:A:GLU:HA	6	0.37
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD2	1	0.37
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD3	1	0.37
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD2	2	0.37
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD3	2	0.37
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD2	9	0.37
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD3	9	0.37
(1,445)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:1:A:GLU:HG2	1:4:A:ALA:H	1	0.37
(1,424)	1:1:A:GLU:HG3	1:4:A:ALA:H	1	0.37
(1,424)	1:1:A:GLU:HG2	1:4:A:ALA:H	2	0.37
(1,424)	1:1:A:GLU:HG3	1:4:A:ALA:H	2	0.37
(1,422)	1:8:A:TYR:HB2	1:9:A:ILE:H	3	0.37
(1,374)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	10	0.37
(1,350)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	4	0.37
(1,350)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	7	0.37
(1,350)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	8	0.37
(1,346)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	0.37
(1,346)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	0.37
(1,346)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.37
(1,136)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	9	0.37
(1,49)	1:6:A:ARG:H	1:6:A:ARG:HB2	6	0.37
(1,35)	1:6:A:ARG:HA	1:6:A:ARG:HG2	3	0.37
(1,14)	1:3:A:GLU:H	1:3:A:GLU:HB3	2	0.37
(1,14)	1:3:A:GLU:H	1:3:A:GLU:HB3	7	0.37
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG2	1	0.37
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG3	1	0.37
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	10	0.36
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	10	0.36
(4,58)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	10	0.36
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	10	0.36
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	10	0.36
(4,58)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	10	0.36
(4,43)	1:7:A:LEU:HB2	1:8:A:TYR:H	10	0.36
(4,39)	1:1:A:GLU:HG2	1:4:A:ALA:H	7	0.36
(4,39)	1:1:A:GLU:HG3	1:4:A:ALA:H	7	0.36
(4,38)	1:3:A:GLU:H	1:5:A:VAL:HB	6	0.36
(4,25)	1:24:A:PRO:HA	1:25:A:SER:H	4	0.36
(4,1)	1:2:A:GLU:HA	1:3:A:GLU:H	5	0.36
(3,606)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	7	0.36
(3,606)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	7	0.36
(3,606)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	7	0.36
(3,528)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	6	0.36
(3,528)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	6	0.36
(3,528)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	6	0.36
(3,384)	1:8:A:TYR:HB2	1:9:A:ILE:H	1	0.36
(3,343)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	5	0.36
(3,115)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	1	0.36
(3,115)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	3	0.36
(3,115)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,115)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	5	0.36
(3,115)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	6	0.36
(3,115)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	7	0.36
(1,678)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	7	0.36
(1,678)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	7	0.36
(1,678)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	7	0.36
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD11	10	0.36
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD12	10	0.36
(1,593)	1:3:A:GLU:HG2	1:7:A:LEU:HD13	10	0.36
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD11	10	0.36
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD12	10	0.36
(1,593)	1:3:A:GLU:HG3	1:7:A:LEU:HD13	10	0.36
(1,585)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	6	0.36
(1,585)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	6	0.36
(1,585)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	6	0.36
(1,460)	1:7:A:LEU:HB2	1:8:A:TYR:H	10	0.36
(1,424)	1:1:A:GLU:HG2	1:4:A:ALA:H	7	0.36
(1,424)	1:1:A:GLU:HG3	1:4:A:ALA:H	7	0.36
(1,422)	1:8:A:TYR:HB2	1:9:A:ILE:H	1	0.36
(1,422)	1:8:A:TYR:HB2	1:9:A:ILE:H	2	0.36
(1,417)	1:3:A:GLU:H	1:5:A:VAL:HB	6	0.36
(1,374)	1:11:A:TRP:HZ3	1:16:A:GLY:HA2	5	0.36
(1,285)	1:24:A:PRO:HA	1:25:A:SER:H	4	0.36
(1,136)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	1	0.36
(1,136)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	3	0.36
(1,136)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	4	0.36
(1,136)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	5	0.36
(1,136)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	6	0.36
(1,136)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	7	0.36
(1,1)	1:2:A:GLU:HA	1:3:A:GLU:H	5	0.36
(4,68)	1:7:A:LEU:HA	1:8:A:TYR:H	2	0.35
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD21	4	0.35
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD22	4	0.35
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD23	4	0.35
(4,52)	1:1:A:GLU:HB2	1:2:A:GLU:HA	5	0.35
(4,43)	1:7:A:LEU:HB2	1:8:A:TYR:H	3	0.35
(4,30)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	0.35
(4,25)	1:24:A:PRO:HA	1:25:A:SER:H	5	0.35
(4,21)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.35
(4,3)	1:3:A:GLU:H	1:3:A:GLU:HB3	5	0.35
(3,528)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	2	0.35
(3,528)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,528)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	2	0.35
(3,384)	1:8:A:TYR:HB2	1:9:A:ILE:H	2	0.35
(3,384)	1:8:A:TYR:HB2	1:9:A:ILE:H	6	0.35
(3,384)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.35
(3,115)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	8	0.35
(3,100)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	10	0.35
(1,665)	1:7:A:LEU:HA	1:8:A:TYR:H	2	0.35
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD21	4	0.35
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD22	4	0.35
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD23	4	0.35
(1,585)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	2	0.35
(1,585)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	2	0.35
(1,585)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	2	0.35
(1,529)	1:1:A:GLU:HB2	1:2:A:GLU:HA	5	0.35
(1,460)	1:7:A:LEU:HB2	1:8:A:TYR:H	3	0.35
(1,422)	1:8:A:TYR:HB2	1:9:A:ILE:H	6	0.35
(1,422)	1:8:A:TYR:HB2	1:9:A:ILE:H	10	0.35
(1,346)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	0.35
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.35
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.35
(1,285)	1:24:A:PRO:HA	1:25:A:SER:H	5	0.35
(1,136)	1:10:A:GLN:HE22	1:10:A:GLN:HG3	8	0.35
(1,125)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	0.35
(1,119)	1:10:A:GLN:HB2	1:10:A:GLN:HG3	10	0.35
(1,14)	1:3:A:GLU:H	1:3:A:GLU:HB3	5	0.35
(4,68)	1:7:A:LEU:HA	1:8:A:TYR:H	3	0.34
(4,68)	1:7:A:LEU:HA	1:8:A:TYR:H	6	0.34
(4,68)	1:7:A:LEU:HA	1:8:A:TYR:H	9	0.34
(4,66)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	4	0.34
(4,66)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	4	0.34
(4,66)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	4	0.34
(4,62)	1:5:A:VAL:HG11	1:9:A:ILE:H	7	0.34
(4,62)	1:5:A:VAL:HG12	1:9:A:ILE:H	7	0.34
(4,62)	1:5:A:VAL:HG13	1:9:A:ILE:H	7	0.34
(4,53)	1:3:A:GLU:HA	1:6:A:ARG:HB2	8	0.34
(4,39)	1:1:A:GLU:HG2	1:4:A:ALA:H	8	0.34
(4,39)	1:1:A:GLU:HG3	1:4:A:ALA:H	8	0.34
(4,30)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	0.34
(4,30)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	0.34
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.34
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.34
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.34
(4,25)	1:24:A:PRO:HA	1:25:A:SER:H	7	0.34
(4,21)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.34
(4,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	1	0.34
(4,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.34
(4,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	7	0.34
(4,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	8	0.34
(3,568)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	2	0.34
(3,384)	1:8:A:TYR:HB2	1:9:A:ILE:H	4	0.34
(1,665)	1:7:A:LEU:HA	1:8:A:TYR:H	3	0.34
(1,665)	1:7:A:LEU:HA	1:8:A:TYR:H	6	0.34
(1,665)	1:7:A:LEU:HA	1:8:A:TYR:H	9	0.34
(1,653)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	4	0.34
(1,653)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	4	0.34
(1,653)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	4	0.34
(1,631)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	2	0.34
(1,613)	1:5:A:VAL:HG11	1:9:A:ILE:H	7	0.34
(1,613)	1:5:A:VAL:HG12	1:9:A:ILE:H	7	0.34
(1,613)	1:5:A:VAL:HG13	1:9:A:ILE:H	7	0.34
(1,534)	1:3:A:GLU:HA	1:6:A:ARG:HB2	8	0.34
(1,424)	1:1:A:GLU:HG2	1:4:A:ALA:H	8	0.34
(1,424)	1:1:A:GLU:HG3	1:4:A:ALA:H	8	0.34
(1,422)	1:8:A:TYR:HB2	1:9:A:ILE:H	4	0.34
(1,346)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	0.34
(1,346)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	0.34
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.34
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.34
(1,285)	1:24:A:PRO:HA	1:25:A:SER:H	7	0.34
(1,125)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.34
(1,124)	1:10:A:GLN:H	1:10:A:GLN:HG2	1	0.34
(1,124)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.34
(1,124)	1:10:A:GLN:H	1:10:A:GLN:HG2	7	0.34
(1,124)	1:10:A:GLN:H	1:10:A:GLN:HG2	8	0.34
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD21	1	0.33
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD22	1	0.33
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD23	1	0.33
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD21	3	0.33
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD22	3	0.33
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD23	3	0.33
(4,62)	1:5:A:VAL:HG11	1:9:A:ILE:H	1	0.33
(4,62)	1:5:A:VAL:HG12	1:9:A:ILE:H	1	0.33
(4,62)	1:5:A:VAL:HG13	1:9:A:ILE:H	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,62)	1:5:A:VAL:HG11	1:9:A:ILE:H	6	0.33
(4,62)	1:5:A:VAL:HG12	1:9:A:ILE:H	6	0.33
(4,62)	1:5:A:VAL:HG13	1:9:A:ILE:H	6	0.33
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.33
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.33
(4,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	4	0.33
(4,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.33
(4,3)	1:3:A:GLU:H	1:3:A:GLU:HB3	8	0.33
(3,602)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	7	0.33
(3,485)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	9	0.33
(3,485)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	9	0.33
(3,480)	1:8:A:TYR:HA	1:24:A:PRO:HB3	1	0.33
(1,673)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	7	0.33
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD21	1	0.33
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD22	1	0.33
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD23	1	0.33
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD21	3	0.33
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD22	3	0.33
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD23	3	0.33
(1,613)	1:5:A:VAL:HG11	1:9:A:ILE:H	1	0.33
(1,613)	1:5:A:VAL:HG12	1:9:A:ILE:H	1	0.33
(1,613)	1:5:A:VAL:HG13	1:9:A:ILE:H	1	0.33
(1,613)	1:5:A:VAL:HG11	1:9:A:ILE:H	6	0.33
(1,613)	1:5:A:VAL:HG12	1:9:A:ILE:H	6	0.33
(1,613)	1:5:A:VAL:HG13	1:9:A:ILE:H	6	0.33
(1,538)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	9	0.33
(1,538)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	9	0.33
(1,532)	1:8:A:TYR:HA	1:24:A:PRO:HB3	1	0.33
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.33
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.33
(1,124)	1:10:A:GLN:H	1:10:A:GLN:HG2	4	0.33
(1,124)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.33
(1,14)	1:3:A:GLU:H	1:3:A:GLU:HB3	8	0.33
(4,68)	1:7:A:LEU:HA	1:8:A:TYR:H	4	0.32
(4,68)	1:7:A:LEU:HA	1:8:A:TYR:H	5	0.32
(4,68)	1:7:A:LEU:HA	1:8:A:TYR:H	7	0.32
(4,68)	1:7:A:LEU:HA	1:8:A:TYR:H	8	0.32
(4,68)	1:7:A:LEU:HA	1:8:A:TYR:H	10	0.32
(4,66)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	3	0.32
(4,66)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	3	0.32
(4,66)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	3	0.32
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD21	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD22	7	0.32
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD23	7	0.32
(4,62)	1:5:A:VAL:HG11	1:9:A:ILE:H	2	0.32
(4,62)	1:5:A:VAL:HG12	1:9:A:ILE:H	2	0.32
(4,62)	1:5:A:VAL:HG13	1:9:A:ILE:H	2	0.32
(4,62)	1:5:A:VAL:HG11	1:9:A:ILE:H	5	0.32
(4,62)	1:5:A:VAL:HG12	1:9:A:ILE:H	5	0.32
(4,62)	1:5:A:VAL:HG13	1:9:A:ILE:H	5	0.32
(4,62)	1:5:A:VAL:HG11	1:9:A:ILE:H	8	0.32
(4,62)	1:5:A:VAL:HG12	1:9:A:ILE:H	8	0.32
(4,62)	1:5:A:VAL:HG13	1:9:A:ILE:H	8	0.32
(4,52)	1:1:A:GLU:HB2	1:2:A:GLU:HA	2	0.32
(4,52)	1:1:A:GLU:HB2	1:2:A:GLU:HA	8	0.32
(4,52)	1:1:A:GLU:HB2	1:2:A:GLU:HA	9	0.32
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD2	4	0.32
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD3	4	0.32
(4,30)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	0.32
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.32
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.32
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.32
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.32
(4,25)	1:24:A:PRO:HA	1:25:A:SER:H	1	0.32
(4,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	5	0.32
(4,10)	1:9:A:ILE:H	1:9:A:ILE:HG12	3	0.32
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD11	3	0.32
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD12	3	0.32
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD13	3	0.32
(3,568)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	3	0.32
(3,480)	1:8:A:TYR:HA	1:24:A:PRO:HB3	2	0.32
(3,423)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	0.32
(3,423)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	0.32
(3,423)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	0.32
(3,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	4	0.32
(3,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	9	0.32
(3,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.32
(1,665)	1:7:A:LEU:HA	1:8:A:TYR:H	4	0.32
(1,665)	1:7:A:LEU:HA	1:8:A:TYR:H	5	0.32
(1,665)	1:7:A:LEU:HA	1:8:A:TYR:H	7	0.32
(1,665)	1:7:A:LEU:HA	1:8:A:TYR:H	8	0.32
(1,665)	1:7:A:LEU:HA	1:8:A:TYR:H	10	0.32
(1,653)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	3	0.32
(1,653)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	3	0.32
(1,631)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	3	0.32
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD21	7	0.32
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD22	7	0.32
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD23	7	0.32
(1,613)	1:5:A:VAL:HG11	1:9:A:ILE:H	2	0.32
(1,613)	1:5:A:VAL:HG12	1:9:A:ILE:H	2	0.32
(1,613)	1:5:A:VAL:HG13	1:9:A:ILE:H	2	0.32
(1,613)	1:5:A:VAL:HG11	1:9:A:ILE:H	5	0.32
(1,613)	1:5:A:VAL:HG12	1:9:A:ILE:H	5	0.32
(1,613)	1:5:A:VAL:HG13	1:9:A:ILE:H	5	0.32
(1,613)	1:5:A:VAL:HG11	1:9:A:ILE:H	8	0.32
(1,613)	1:5:A:VAL:HG12	1:9:A:ILE:H	8	0.32
(1,613)	1:5:A:VAL:HG13	1:9:A:ILE:H	8	0.32
(1,532)	1:8:A:TYR:HA	1:24:A:PRO:HB3	2	0.32
(1,529)	1:1:A:GLU:HB2	1:2:A:GLU:HA	2	0.32
(1,529)	1:1:A:GLU:HB2	1:2:A:GLU:HA	8	0.32
(1,529)	1:1:A:GLU:HB2	1:2:A:GLU:HA	9	0.32
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD2	4	0.32
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD3	4	0.32
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	0.32
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	0.32
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	0.32
(1,346)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	0.32
(1,315)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	4	0.32
(1,315)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	9	0.32
(1,315)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	10	0.32
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.32
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.32
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.32
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.32
(1,285)	1:24:A:PRO:HA	1:25:A:SER:H	1	0.32
(1,124)	1:10:A:GLN:H	1:10:A:GLN:HG2	5	0.32
(1,68)	1:9:A:ILE:H	1:9:A:ILE:HG12	3	0.32
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD11	3	0.32
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD12	3	0.32
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD13	3	0.32
(4,68)	1:7:A:LEU:HA	1:8:A:TYR:H	1	0.31
(4,66)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	6	0.31
(4,66)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	6	0.31
(4,66)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	6	0.31
(4,66)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,66)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	10	0.31
(4,66)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	10	0.31
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD21	8	0.31
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD22	8	0.31
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD23	8	0.31
(4,53)	1:3:A:GLU:HA	1:6:A:ARG:HB2	7	0.31
(4,52)	1:1:A:GLU:HB2	1:2:A:GLU:HA	1	0.31
(4,52)	1:1:A:GLU:HB2	1:2:A:GLU:HA	7	0.31
(4,40)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.31
(4,39)	1:1:A:GLU:HG2	1:4:A:ALA:H	5	0.31
(4,39)	1:1:A:GLU:HG3	1:4:A:ALA:H	5	0.31
(4,30)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	0.31
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.31
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.31
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.31
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.31
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.31
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.31
(4,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	10	0.31
(4,3)	1:3:A:GLU:H	1:3:A:GLU:HB3	9	0.31
(4,1)	1:2:A:GLU:HA	1:3:A:GLU:H	6	0.31
(3,606)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	4	0.31
(3,606)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	4	0.31
(3,606)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	4	0.31
(3,568)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	6	0.31
(3,555)	1:2:A:GLU:HB2	1:4:A:ALA:H	3	0.31
(3,555)	1:2:A:GLU:HB3	1:4:A:ALA:H	3	0.31
(3,555)	1:2:A:GLU:HB2	1:4:A:ALA:H	4	0.31
(3,555)	1:2:A:GLU:HB3	1:4:A:ALA:H	4	0.31
(3,480)	1:8:A:TYR:HA	1:24:A:PRO:HB3	5	0.31
(3,423)	1:5:A:VAL:HG21	1:6:A:ARG:H	3	0.31
(3,423)	1:5:A:VAL:HG22	1:6:A:ARG:H	3	0.31
(3,423)	1:5:A:VAL:HG23	1:6:A:ARG:H	3	0.31
(3,423)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.31
(3,423)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.31
(3,423)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.31
(3,302)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	8	0.31
(3,302)	1:11:A:TRP:HE1	1:21:A:ARG:HG3	8	0.31
(3,293)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	4	0.31
(3,293)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	4	0.31
(3,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	3	0.31
(3,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,678)	1:7:A:LEU:HD11	1:24:A:PRO:HB3	4	0.31
(1,678)	1:7:A:LEU:HD12	1:24:A:PRO:HB3	4	0.31
(1,678)	1:7:A:LEU:HD13	1:24:A:PRO:HB3	4	0.31
(1,665)	1:7:A:LEU:HA	1:8:A:TYR:H	1	0.31
(1,653)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	6	0.31
(1,653)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	6	0.31
(1,653)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	6	0.31
(1,653)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	10	0.31
(1,653)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	10	0.31
(1,653)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	10	0.31
(1,631)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	6	0.31
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD21	8	0.31
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD22	8	0.31
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD23	8	0.31
(1,617)	1:2:A:GLU:HB2	1:4:A:ALA:H	3	0.31
(1,617)	1:2:A:GLU:HB3	1:4:A:ALA:H	3	0.31
(1,617)	1:2:A:GLU:HB2	1:4:A:ALA:H	4	0.31
(1,617)	1:2:A:GLU:HB3	1:4:A:ALA:H	4	0.31
(1,534)	1:3:A:GLU:HA	1:6:A:ARG:HB2	7	0.31
(1,532)	1:8:A:TYR:HA	1:24:A:PRO:HB3	5	0.31
(1,529)	1:1:A:GLU:HB2	1:2:A:GLU:HA	1	0.31
(1,529)	1:1:A:GLU:HB2	1:2:A:GLU:HA	7	0.31
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:H	3	0.31
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:H	3	0.31
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:H	3	0.31
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:H	10	0.31
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:H	10	0.31
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:H	10	0.31
(1,439)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.31
(1,424)	1:1:A:GLU:HG2	1:4:A:ALA:H	5	0.31
(1,424)	1:1:A:GLU:HG3	1:4:A:ALA:H	5	0.31
(1,346)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	0.31
(1,331)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	8	0.31
(1,331)	1:11:A:TRP:HE1	1:21:A:ARG:HG3	8	0.31
(1,322)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	4	0.31
(1,322)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	4	0.31
(1,315)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	3	0.31
(1,315)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	5	0.31
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.31
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.31
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.31
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.31
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.31
(1,35)	1:6:A:ARG:HA	1:6:A:ARG:HG2	10	0.31
(1,14)	1:3:A:GLU:H	1:3:A:GLU:HB3	9	0.31
(1,1)	1:2:A:GLU:HA	1:3:A:GLU:H	6	0.31
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD21	2	0.3
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD22	2	0.3
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD23	2	0.3
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.3
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.3
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.3
(4,27)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.3
(3,555)	1:2:A:GLU:HB2	1:4:A:ALA:H	10	0.3
(3,555)	1:2:A:GLU:HB3	1:4:A:ALA:H	10	0.3
(3,499)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	2	0.3
(3,499)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	10	0.3
(3,491)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	5	0.3
(3,480)	1:8:A:TYR:HA	1:24:A:PRO:HB3	8	0.3
(2,1)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	3	0.3
(2,1)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	3	0.3
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD21	2	0.3
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD22	2	0.3
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD23	2	0.3
(1,617)	1:2:A:GLU:HB2	1:4:A:ALA:H	10	0.3
(1,617)	1:2:A:GLU:HB3	1:4:A:ALA:H	10	0.3
(1,553)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	2	0.3
(1,553)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	10	0.3
(1,545)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	5	0.3
(1,532)	1:8:A:TYR:HA	1:24:A:PRO:HB3	8	0.3
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.3
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.3
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.3
(1,306)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.3
(4,66)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	1	0.29
(4,66)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	1	0.29
(4,66)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	1	0.29
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD21	6	0.29
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD22	6	0.29
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD23	6	0.29
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD2	7	0.29
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD3	7	0.29
(4,38)	1:3:A:GLU:H	1:5:A:VAL:HB	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,38)	1:3:A:GLU:H	1:5:A:VAL:HB	10	0.29
(4,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	2	0.29
(1,653)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	1	0.29
(1,653)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	1	0.29
(1,653)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	1	0.29
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD21	5	0.29
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD22	5	0.29
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD23	5	0.29
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD21	6	0.29
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD22	6	0.29
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD23	6	0.29
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD2	7	0.29
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD3	7	0.29
(1,417)	1:3:A:GLU:H	1:5:A:VAL:HB	4	0.29
(1,417)	1:3:A:GLU:H	1:5:A:VAL:HB	10	0.29
(1,124)	1:10:A:GLN:H	1:10:A:GLN:HG2	2	0.29
(4,66)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	5	0.28
(4,66)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	5	0.28
(4,66)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	5	0.28
(4,66)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	7	0.28
(4,66)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	7	0.28
(4,66)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	7	0.28
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD21	5	0.28
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD22	5	0.28
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD23	5	0.28
(4,54)	1:16:A:GLY:HA2	1:19:A:SER:HB3	2	0.28
(4,50)	1:7:A:LEU:HA	1:11:A:TRP:H	5	0.28
(4,38)	1:3:A:GLU:H	1:5:A:VAL:HB	3	0.28
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	4	0.28
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	4	0.28
(4,24)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	7	0.28
(3,499)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	5	0.28
(3,384)	1:8:A:TYR:HB2	1:9:A:ILE:H	9	0.28
(3,302)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	7	0.28
(3,302)	1:11:A:TRP:HE1	1:21:A:ARG:HG3	7	0.28
(3,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	1	0.28
(3,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	6	0.28
(1,653)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	5	0.28
(1,653)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	5	0.28
(1,653)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	5	0.28
(1,653)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	7	0.28
(1,653)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	7	0.28
(1,553)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	5	0.28
(1,542)	1:16:A:GLY:HA2	1:19:A:SER:HB3	2	0.28
(1,494)	1:7:A:LEU:HA	1:11:A:TRP:H	5	0.28
(1,422)	1:8:A:TYR:HB2	1:9:A:ILE:H	9	0.28
(1,417)	1:3:A:GLU:H	1:5:A:VAL:HB	3	0.28
(1,331)	1:11:A:TRP:HE1	1:21:A:ARG:HG2	7	0.28
(1,331)	1:11:A:TRP:HE1	1:21:A:ARG:HG3	7	0.28
(1,315)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	1	0.28
(1,315)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	6	0.28
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	4	0.28
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	4	0.28
(1,248)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	7	0.28
(4,72)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	2	0.27
(4,72)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	2	0.27
(4,72)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	2	0.27
(4,53)	1:3:A:GLU:HA	1:6:A:ARG:HB2	5	0.27
(4,50)	1:7:A:LEU:HA	1:11:A:TRP:H	6	0.27
(4,50)	1:7:A:LEU:HA	1:11:A:TRP:H	10	0.27
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD2	5	0.27
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD3	5	0.27
(4,40)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.27
(4,24)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	8	0.27
(4,10)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.27
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG2	3	0.27
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG3	3	0.27
(3,128)	1:13:A:LYS:HA	1:13:A:LYS:HG3	10	0.27
(2,1)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	6	0.27
(2,1)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	6	0.27
(1,681)	1:12:A:LEU:HD11	1:16:A:GLY:HA2	2	0.27
(1,681)	1:12:A:LEU:HD12	1:16:A:GLY:HA2	2	0.27
(1,681)	1:12:A:LEU:HD13	1:16:A:GLY:HA2	2	0.27
(1,534)	1:3:A:GLU:HA	1:6:A:ARG:HB2	5	0.27
(1,494)	1:7:A:LEU:HA	1:11:A:TRP:H	6	0.27
(1,494)	1:7:A:LEU:HA	1:11:A:TRP:H	10	0.27
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD2	5	0.27
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD3	5	0.27
(1,439)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.27
(1,248)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	8	0.27
(1,149)	1:13:A:LYS:HA	1:13:A:LYS:HG3	10	0.27
(1,68)	1:9:A:ILE:H	1:9:A:ILE:HG12	10	0.27
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG2	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG3	3	0.27
(4,71)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	9	0.26
(4,71)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	9	0.26
(4,71)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	9	0.26
(4,66)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	8	0.26
(4,66)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	8	0.26
(4,66)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	8	0.26
(4,50)	1:7:A:LEU:HA	1:11:A:TRP:H	4	0.26
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD2	3	0.26
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD3	3	0.26
(4,34)	1:8:A:TYR:HD1	1:12:A:LEU:H	3	0.26
(4,34)	1:8:A:TYR:HD2	1:12:A:LEU:H	3	0.26
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	1	0.26
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	1	0.26
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	6	0.26
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	6	0.26
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	7	0.26
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	7	0.26
(4,10)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.26
(4,10)	1:9:A:ILE:H	1:9:A:ILE:HG12	5	0.26
(3,602)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	8	0.26
(3,561)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	9	0.26
(3,499)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	3	0.26
(3,344)	1:21:A:ARG:HD3	1:21:A:ARG:HH11	3	0.26
(3,344)	1:21:A:ARG:HD3	1:21:A:ARG:HH12	3	0.26
(3,344)	1:21:A:ARG:HD3	1:21:A:ARG:HH11	10	0.26
(3,344)	1:21:A:ARG:HD3	1:21:A:ARG:HH12	10	0.26
(3,293)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	1	0.26
(3,293)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	1	0.26
(3,293)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	5	0.26
(3,293)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	5	0.26
(3,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.26
(3,128)	1:13:A:LYS:HA	1:13:A:LYS:HG3	8	0.26
(2,1)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	9	0.26
(2,1)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	9	0.26
(2,1)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	10	0.26
(2,1)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	10	0.26
(1,675)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	9	0.26
(1,675)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	9	0.26
(1,675)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	9	0.26
(1,673)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	8	0.26
(1,653)	1:7:A:LEU:HD11	1:10:A:GLN:HB3	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:7:A:LEU:HD12	1:10:A:GLN:HB3	8	0.26
(1,653)	1:7:A:LEU:HD13	1:10:A:GLN:HB3	8	0.26
(1,624)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	9	0.26
(1,553)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	3	0.26
(1,494)	1:7:A:LEU:HA	1:11:A:TRP:H	4	0.26
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD2	3	0.26
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD3	3	0.26
(1,389)	1:8:A:TYR:HD1	1:12:A:LEU:H	3	0.26
(1,389)	1:8:A:TYR:HD2	1:12:A:LEU:H	3	0.26
(1,375)	1:21:A:ARG:HD3	1:21:A:ARG:HH11	3	0.26
(1,375)	1:21:A:ARG:HD3	1:21:A:ARG:HH12	3	0.26
(1,375)	1:21:A:ARG:HD3	1:21:A:ARG:HH11	10	0.26
(1,375)	1:21:A:ARG:HD3	1:21:A:ARG:HH12	10	0.26
(1,322)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	1	0.26
(1,322)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	1	0.26
(1,322)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	5	0.26
(1,322)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	5	0.26
(1,315)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.26
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	1	0.26
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	1	0.26
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	6	0.26
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	6	0.26
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	7	0.26
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	7	0.26
(1,149)	1:13:A:LYS:HA	1:13:A:LYS:HG3	8	0.26
(1,68)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.26
(1,68)	1:9:A:ILE:H	1:9:A:ILE:HG12	5	0.26
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD21	9	0.25
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD22	9	0.25
(4,63)	1:6:A:ARG:H	1:7:A:LEU:HD23	9	0.25
(4,50)	1:7:A:LEU:HA	1:11:A:TRP:H	8	0.25
(4,40)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.25
(4,40)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.25
(4,40)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.25
(4,10)	1:9:A:ILE:H	1:9:A:ILE:HG12	8	0.25
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD11	8	0.25
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD12	8	0.25
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD13	8	0.25
(4,3)	1:3:A:GLU:H	1:3:A:GLU:HB3	6	0.25
(3,568)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	4	0.25
(3,458)	1:23:A:PRO:HB3	1:25:A:SER:H	3	0.25
(3,357)	1:8:A:TYR:HD1	1:11:A:TRP:H	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,357)	1:8:A:TYR:HD2	1:11:A:TRP:H	3	0.25
(3,211)	1:21:A:ARG:HA	1:22:A:PRO:HD2	7	0.25
(3,211)	1:21:A:ARG:HA	1:22:A:PRO:HD2	8	0.25
(1,631)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	4	0.25
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD21	9	0.25
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD22	9	0.25
(1,620)	1:6:A:ARG:H	1:7:A:LEU:HD23	9	0.25
(1,508)	1:23:A:PRO:HB3	1:25:A:SER:H	3	0.25
(1,494)	1:7:A:LEU:HA	1:11:A:TRP:H	8	0.25
(1,439)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.25
(1,439)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.25
(1,439)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.25
(1,391)	1:8:A:TYR:HD1	1:11:A:TRP:H	3	0.25
(1,391)	1:8:A:TYR:HD2	1:11:A:TRP:H	3	0.25
(1,234)	1:21:A:ARG:HA	1:22:A:PRO:HD2	7	0.25
(1,234)	1:21:A:ARG:HA	1:22:A:PRO:HD2	8	0.25
(1,68)	1:9:A:ILE:H	1:9:A:ILE:HG12	8	0.25
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD11	8	0.25
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD12	8	0.25
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD13	8	0.25
(1,14)	1:3:A:GLU:H	1:3:A:GLU:HB3	6	0.25
(4,71)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	6	0.24
(4,71)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	6	0.24
(4,71)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	6	0.24
(4,69)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	6	0.24
(4,69)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	6	0.24
(4,69)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	9	0.24
(4,69)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	9	0.24
(4,62)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	0.24
(4,62)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	0.24
(4,62)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	0.24
(4,53)	1:3:A:GLU:HA	1:6:A:ARG:HB2	1	0.24
(4,40)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.24
(4,40)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.24
(4,39)	1:1:A:GLU:HG2	1:4:A:ALA:H	6	0.24
(4,39)	1:1:A:GLU:HG3	1:4:A:ALA:H	6	0.24
(4,38)	1:3:A:GLU:H	1:5:A:VAL:HB	2	0.24
(4,38)	1:3:A:GLU:H	1:5:A:VAL:HB	5	0.24
(4,10)	1:9:A:ILE:H	1:9:A:ILE:HG12	4	0.24
(4,9)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.24
(4,9)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.24
(4,9)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,9)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.24
(4,9)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.24
(4,9)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD11	1	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD12	1	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD13	1	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD11	5	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD12	5	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD13	5	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.24
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.24
(3,602)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	5	0.24
(3,485)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	4	0.24
(3,485)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	4	0.24
(3,480)	1:8:A:TYR:HA	1:24:A:PRO:HB3	7	0.24
(3,423)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.24
(3,423)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.24
(3,423)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.24
(3,293)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	2	0.24
(3,293)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	2	0.24
(3,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	8	0.24
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE1	1	0.24
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE2	1	0.24
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE1	8	0.24
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE2	8	0.24
(1,675)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	6	0.24
(1,675)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	6	0.24
(1,675)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	6	0.24
(1,673)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	5	0.24
(1,669)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	6	0.24
(1,669)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	6	0.24
(1,669)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	9	0.24
(1,669)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	9	0.24
(1,613)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	0.24
(1,613)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	0.24
(1,613)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	0.24
(1,538)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	4	0.24
(1,538)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:3:A:GLU:HA	1:6:A:ARG:HB2	1	0.24
(1,532)	1:8:A:TYR:HA	1:24:A:PRO:HB3	7	0.24
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.24
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.24
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.24
(1,439)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.24
(1,439)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.24
(1,424)	1:1:A:GLU:HG2	1:4:A:ALA:H	6	0.24
(1,424)	1:1:A:GLU:HG3	1:4:A:ALA:H	6	0.24
(1,417)	1:3:A:GLU:H	1:5:A:VAL:HB	2	0.24
(1,417)	1:3:A:GLU:H	1:5:A:VAL:HB	5	0.24
(1,322)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	2	0.24
(1,322)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	2	0.24
(1,315)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	8	0.24
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE1	1	0.24
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE2	1	0.24
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE1	8	0.24
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE2	8	0.24
(1,149)	1:13:A:LYS:HA	1:13:A:LYS:HG3	3	0.24
(1,68)	1:9:A:ILE:H	1:9:A:ILE:HG12	4	0.24
(1,60)	1:9:A:ILE:HB	1:9:A:ILE:HG12	1	0.24
(1,60)	1:9:A:ILE:HB	1:9:A:ILE:HG12	3	0.24
(1,60)	1:9:A:ILE:HB	1:9:A:ILE:HG12	4	0.24
(1,60)	1:9:A:ILE:HB	1:9:A:ILE:HG12	5	0.24
(1,60)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.24
(1,60)	1:9:A:ILE:HB	1:9:A:ILE:HG12	10	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD11	1	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD12	1	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD13	1	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD11	5	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD12	5	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD13	5	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.24
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.24
(4,53)	1:3:A:GLU:HA	1:6:A:ARG:HB2	3	0.23
(4,50)	1:7:A:LEU:HA	1:11:A:TRP:H	1	0.23
(4,50)	1:7:A:LEU:HA	1:11:A:TRP:H	3	0.23
(4,50)	1:7:A:LEU:HA	1:11:A:TRP:H	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,40)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.23
(4,40)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.23
(4,40)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.23
(4,38)	1:3:A:GLU:H	1:5:A:VAL:HB	8	0.23
(4,23)	1:19:A:SER:HA	1:19:A:SER:HB3	1	0.23
(4,23)	1:19:A:SER:HA	1:19:A:SER:HB3	3	0.23
(4,20)	1:10:A:GLN:H	1:10:A:GLN:HG2	9	0.23
(4,9)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.23
(4,9)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.23
(4,9)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.23
(4,9)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.23
(3,602)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	2	0.23
(3,528)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	4	0.23
(3,528)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	4	0.23
(3,528)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	4	0.23
(3,499)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	1	0.23
(3,499)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	6	0.23
(3,399)	1:16:A:GLY:H	1:17:A:PRO:HD2	2	0.23
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE1	2	0.23
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE2	2	0.23
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE1	5	0.23
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE2	5	0.23
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE1	7	0.23
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE2	7	0.23
(3,224)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	4	0.23
(3,224)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	5	0.23
(3,224)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.23
(3,128)	1:13:A:LYS:HA	1:13:A:LYS:HG3	3	0.23
(1,673)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	2	0.23
(1,585)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	4	0.23
(1,585)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	4	0.23
(1,585)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	4	0.23
(1,553)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	1	0.23
(1,553)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	6	0.23
(1,534)	1:3:A:GLU:HA	1:6:A:ARG:HB2	3	0.23
(1,494)	1:7:A:LEU:HA	1:11:A:TRP:H	1	0.23
(1,494)	1:7:A:LEU:HA	1:11:A:TRP:H	3	0.23
(1,494)	1:7:A:LEU:HA	1:11:A:TRP:H	7	0.23
(1,439)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.23
(1,439)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.23
(1,439)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.23
(1,438)	1:16:A:GLY:H	1:17:A:PRO:HD2	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:3:A:GLU:H	1:5:A:VAL:HB	8	0.23
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE1	2	0.23
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE2	2	0.23
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE1	5	0.23
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE2	5	0.23
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE1	7	0.23
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE2	7	0.23
(1,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	4	0.23
(1,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	5	0.23
(1,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.23
(1,205)	1:19:A:SER:HA	1:19:A:SER:HB3	1	0.23
(1,205)	1:19:A:SER:HA	1:19:A:SER:HB3	3	0.23
(1,124)	1:10:A:GLN:H	1:10:A:GLN:HG2	9	0.23
(1,60)	1:9:A:ILE:HB	1:9:A:ILE:HG12	2	0.23
(1,60)	1:9:A:ILE:HB	1:9:A:ILE:HG12	6	0.23
(1,60)	1:9:A:ILE:HB	1:9:A:ILE:HG12	7	0.23
(1,60)	1:9:A:ILE:HB	1:9:A:ILE:HG12	9	0.23
(4,71)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	5	0.22
(4,71)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	5	0.22
(4,71)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	5	0.22
(4,71)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	7	0.22
(4,71)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	7	0.22
(4,71)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	7	0.22
(4,69)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	10	0.22
(4,69)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	10	0.22
(4,62)	1:5:A:VAL:HG11	1:9:A:ILE:H	4	0.22
(4,62)	1:5:A:VAL:HG12	1:9:A:ILE:H	4	0.22
(4,62)	1:5:A:VAL:HG13	1:9:A:ILE:H	4	0.22
(4,50)	1:7:A:LEU:HA	1:11:A:TRP:H	2	0.22
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	2	0.22
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	2	0.22
(4,23)	1:19:A:SER:HA	1:19:A:SER:HB3	7	0.22
(4,23)	1:19:A:SER:HA	1:19:A:SER:HB3	8	0.22
(3,528)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	1	0.22
(3,528)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	1	0.22
(3,528)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	1	0.22
(3,499)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	9	0.22
(3,423)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	0.22
(3,423)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	0.22
(3,423)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	0.22
(3,287)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	7	0.22
(1,675)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	5	0.22
(1,675)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	5	0.22
(1,675)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	7	0.22
(1,675)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	7	0.22
(1,675)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	7	0.22
(1,669)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	10	0.22
(1,669)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	10	0.22
(1,613)	1:5:A:VAL:HG11	1:9:A:ILE:H	4	0.22
(1,613)	1:5:A:VAL:HG12	1:9:A:ILE:H	4	0.22
(1,613)	1:5:A:VAL:HG13	1:9:A:ILE:H	4	0.22
(1,585)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	1	0.22
(1,585)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	1	0.22
(1,585)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	1	0.22
(1,553)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	9	0.22
(1,494)	1:7:A:LEU:HA	1:11:A:TRP:H	2	0.22
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	0.22
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	0.22
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	0.22
(1,315)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	7	0.22
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	2	0.22
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	2	0.22
(1,205)	1:19:A:SER:HA	1:19:A:SER:HB3	7	0.22
(1,205)	1:19:A:SER:HA	1:19:A:SER:HB3	8	0.22
(1,205)	1:19:A:SER:HA	1:19:A:SER:HB3	10	0.22
(4,71)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	1	0.21
(4,71)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	1	0.21
(4,71)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	1	0.21
(4,71)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	8	0.21
(4,71)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	8	0.21
(4,71)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	8	0.21
(4,53)	1:3:A:GLU:HA	1:6:A:ARG:HB2	6	0.21
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	5	0.21
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	5	0.21
(4,23)	1:19:A:SER:HA	1:19:A:SER:HB3	4	0.21
(4,23)	1:19:A:SER:HA	1:19:A:SER:HB3	6	0.21
(4,23)	1:19:A:SER:HA	1:19:A:SER:HB3	9	0.21
(4,23)	1:19:A:SER:HA	1:19:A:SER:HB3	10	0.21
(4,10)	1:9:A:ILE:H	1:9:A:ILE:HG12	7	0.21
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD11	2	0.21
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD12	2	0.21
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD13	2	0.21
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.21
(3,602)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	1	0.21
(3,568)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	5	0.21
(3,561)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.21
(3,553)	1:8:A:TYR:H	1:24:A:PRO:HG2	4	0.21
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	3	0.21
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	3	0.21
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	3	0.21
(3,496)	1:23:A:PRO:HA	1:24:A:PRO:HD2	7	0.21
(3,485)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	5	0.21
(3,485)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	5	0.21
(3,480)	1:8:A:TYR:HA	1:24:A:PRO:HB3	3	0.21
(3,437)	1:10:A:GLN:HG2	1:11:A:TRP:H	5	0.21
(3,437)	1:10:A:GLN:HG2	1:11:A:TRP:H	9	0.21
(3,423)	1:5:A:VAL:HG21	1:6:A:ARG:H	1	0.21
(3,423)	1:5:A:VAL:HG22	1:6:A:ARG:H	1	0.21
(3,423)	1:5:A:VAL:HG23	1:6:A:ARG:H	1	0.21
(3,407)	1:12:A:LEU:HD11	1:16:A:GLY:H	4	0.21
(3,407)	1:12:A:LEU:HD12	1:16:A:GLY:H	4	0.21
(3,407)	1:12:A:LEU:HD13	1:16:A:GLY:H	4	0.21
(1,675)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	1	0.21
(1,675)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	1	0.21
(1,675)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	1	0.21
(1,675)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	8	0.21
(1,675)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	8	0.21
(1,675)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	8	0.21
(1,673)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	1	0.21
(1,631)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	5	0.21
(1,624)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	10	0.21
(1,615)	1:8:A:TYR:H	1:24:A:PRO:HG2	4	0.21
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	3	0.21
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	3	0.21
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	3	0.21
(1,550)	1:23:A:PRO:HA	1:24:A:PRO:HD2	7	0.21
(1,538)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	5	0.21
(1,538)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	5	0.21
(1,534)	1:3:A:GLU:HA	1:6:A:ARG:HB2	6	0.21
(1,532)	1:8:A:TYR:HA	1:24:A:PRO:HB3	3	0.21
(1,486)	1:10:A:GLN:HG2	1:11:A:TRP:H	5	0.21
(1,486)	1:10:A:GLN:HG2	1:11:A:TRP:H	9	0.21
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:H	1	0.21
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:H	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:H	1	0.21
(1,449)	1:12:A:LEU:HD11	1:16:A:GLY:H	4	0.21
(1,449)	1:12:A:LEU:HD12	1:16:A:GLY:H	4	0.21
(1,449)	1:12:A:LEU:HD13	1:16:A:GLY:H	4	0.21
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	5	0.21
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	5	0.21
(1,205)	1:19:A:SER:HA	1:19:A:SER:HB3	4	0.21
(1,205)	1:19:A:SER:HA	1:19:A:SER:HB3	6	0.21
(1,205)	1:19:A:SER:HA	1:19:A:SER:HB3	9	0.21
(1,68)	1:9:A:ILE:H	1:9:A:ILE:HG12	7	0.21
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD11	2	0.21
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD12	2	0.21
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD13	2	0.21
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.21
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.21
(4,71)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	2	0.2
(4,71)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	2	0.2
(4,71)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	2	0.2
(4,50)	1:7:A:LEU:HA	1:11:A:TRP:H	9	0.2
(4,44)	1:7:A:LEU:HD11	1:8:A:TYR:H	9	0.2
(4,44)	1:7:A:LEU:HD12	1:8:A:TYR:H	9	0.2
(4,44)	1:7:A:LEU:HD13	1:8:A:TYR:H	9	0.2
(4,34)	1:8:A:TYR:HD1	1:12:A:LEU:H	2	0.2
(4,34)	1:8:A:TYR:HD2	1:12:A:LEU:H	2	0.2
(4,34)	1:8:A:TYR:HD1	1:12:A:LEU:H	6	0.2
(4,34)	1:8:A:TYR:HD2	1:12:A:LEU:H	6	0.2
(4,34)	1:8:A:TYR:HD1	1:12:A:LEU:H	10	0.2
(4,34)	1:8:A:TYR:HD2	1:12:A:LEU:H	10	0.2
(4,10)	1:9:A:ILE:H	1:9:A:ILE:HG12	6	0.2
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD11	6	0.2
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD12	6	0.2
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD13	6	0.2
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.2
(4,2)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.2
(3,591)	1:2:A:GLU:HG3	1:4:A:ALA:H	10	0.2
(3,491)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	3	0.2
(3,491)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	4	0.2
(3,485)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	10	0.2
(3,485)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	10	0.2
(3,437)	1:10:A:GLN:HG2	1:11:A:TRP:H	2	0.2
(3,437)	1:10:A:GLN:HG2	1:11:A:TRP:H	6	0.2
(3,423)	1:5:A:VAL:HG21	1:6:A:ARG:H	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,423)	1:5:A:VAL:HG22	1:6:A:ARG:H	8	0.2
(3,423)	1:5:A:VAL:HG23	1:6:A:ARG:H	8	0.2
(3,407)	1:12:A:LEU:HD11	1:16:A:GLY:H	1	0.2
(3,407)	1:12:A:LEU:HD12	1:16:A:GLY:H	1	0.2
(3,407)	1:12:A:LEU:HD13	1:16:A:GLY:H	1	0.2
(3,407)	1:12:A:LEU:HD11	1:16:A:GLY:H	3	0.2
(3,407)	1:12:A:LEU:HD12	1:16:A:GLY:H	3	0.2
(3,407)	1:12:A:LEU:HD13	1:16:A:GLY:H	3	0.2
(3,407)	1:12:A:LEU:HD11	1:16:A:GLY:H	5	0.2
(3,407)	1:12:A:LEU:HD12	1:16:A:GLY:H	5	0.2
(3,407)	1:12:A:LEU:HD13	1:16:A:GLY:H	5	0.2
(3,407)	1:12:A:LEU:HD11	1:16:A:GLY:H	6	0.2
(3,407)	1:12:A:LEU:HD12	1:16:A:GLY:H	6	0.2
(3,407)	1:12:A:LEU:HD13	1:16:A:GLY:H	6	0.2
(3,407)	1:12:A:LEU:HD11	1:16:A:GLY:H	7	0.2
(3,407)	1:12:A:LEU:HD12	1:16:A:GLY:H	7	0.2
(3,407)	1:12:A:LEU:HD13	1:16:A:GLY:H	7	0.2
(3,407)	1:12:A:LEU:HD11	1:16:A:GLY:H	8	0.2
(3,407)	1:12:A:LEU:HD12	1:16:A:GLY:H	8	0.2
(3,407)	1:12:A:LEU:HD13	1:16:A:GLY:H	8	0.2
(3,407)	1:12:A:LEU:HD11	1:16:A:GLY:H	9	0.2
(3,407)	1:12:A:LEU:HD12	1:16:A:GLY:H	9	0.2
(3,407)	1:12:A:LEU:HD13	1:16:A:GLY:H	9	0.2
(3,357)	1:8:A:TYR:HD1	1:11:A:TRP:H	7	0.2
(3,357)	1:8:A:TYR:HD2	1:11:A:TRP:H	7	0.2
(3,224)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	7	0.2
(3,224)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	8	0.2
(3,108)	1:10:A:GLN:HA	1:10:A:GLN:HE21	10	0.2
(3,33)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	6	0.2
(1,675)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	2	0.2
(1,675)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	2	0.2
(1,675)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	2	0.2
(1,658)	1:2:A:GLU:HG3	1:4:A:ALA:H	10	0.2
(1,545)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	3	0.2
(1,545)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	4	0.2
(1,538)	1:21:A:ARG:HG2	1:22:A:PRO:HD3	10	0.2
(1,538)	1:21:A:ARG:HG3	1:22:A:PRO:HD3	10	0.2
(1,494)	1:7:A:LEU:HA	1:11:A:TRP:H	9	0.2
(1,486)	1:10:A:GLN:HG2	1:11:A:TRP:H	2	0.2
(1,486)	1:10:A:GLN:HG2	1:11:A:TRP:H	6	0.2
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:H	8	0.2
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:H	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:H	8	0.2
(1,463)	1:7:A:LEU:HD11	1:8:A:TYR:H	9	0.2
(1,463)	1:7:A:LEU:HD12	1:8:A:TYR:H	9	0.2
(1,463)	1:7:A:LEU:HD13	1:8:A:TYR:H	9	0.2
(1,449)	1:12:A:LEU:HD11	1:16:A:GLY:H	1	0.2
(1,449)	1:12:A:LEU:HD12	1:16:A:GLY:H	1	0.2
(1,449)	1:12:A:LEU:HD13	1:16:A:GLY:H	1	0.2
(1,449)	1:12:A:LEU:HD11	1:16:A:GLY:H	3	0.2
(1,449)	1:12:A:LEU:HD12	1:16:A:GLY:H	3	0.2
(1,449)	1:12:A:LEU:HD13	1:16:A:GLY:H	3	0.2
(1,449)	1:12:A:LEU:HD11	1:16:A:GLY:H	5	0.2
(1,449)	1:12:A:LEU:HD12	1:16:A:GLY:H	5	0.2
(1,449)	1:12:A:LEU:HD13	1:16:A:GLY:H	5	0.2
(1,449)	1:12:A:LEU:HD11	1:16:A:GLY:H	6	0.2
(1,449)	1:12:A:LEU:HD12	1:16:A:GLY:H	6	0.2
(1,449)	1:12:A:LEU:HD13	1:16:A:GLY:H	6	0.2
(1,449)	1:12:A:LEU:HD11	1:16:A:GLY:H	7	0.2
(1,449)	1:12:A:LEU:HD12	1:16:A:GLY:H	7	0.2
(1,449)	1:12:A:LEU:HD13	1:16:A:GLY:H	7	0.2
(1,449)	1:12:A:LEU:HD11	1:16:A:GLY:H	8	0.2
(1,449)	1:12:A:LEU:HD12	1:16:A:GLY:H	8	0.2
(1,449)	1:12:A:LEU:HD13	1:16:A:GLY:H	8	0.2
(1,449)	1:12:A:LEU:HD11	1:16:A:GLY:H	9	0.2
(1,449)	1:12:A:LEU:HD12	1:16:A:GLY:H	9	0.2
(1,449)	1:12:A:LEU:HD13	1:16:A:GLY:H	9	0.2
(1,391)	1:8:A:TYR:HD1	1:11:A:TRP:H	7	0.2
(1,391)	1:8:A:TYR:HD2	1:11:A:TRP:H	7	0.2
(1,389)	1:8:A:TYR:HD1	1:12:A:LEU:H	2	0.2
(1,389)	1:8:A:TYR:HD2	1:12:A:LEU:H	2	0.2
(1,389)	1:8:A:TYR:HD1	1:12:A:LEU:H	6	0.2
(1,389)	1:8:A:TYR:HD2	1:12:A:LEU:H	6	0.2
(1,389)	1:8:A:TYR:HD1	1:12:A:LEU:H	10	0.2
(1,389)	1:8:A:TYR:HD2	1:12:A:LEU:H	10	0.2
(1,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	7	0.2
(1,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	8	0.2
(1,129)	1:10:A:GLN:HA	1:10:A:GLN:HE21	10	0.2
(1,68)	1:9:A:ILE:H	1:9:A:ILE:HG12	6	0.2
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD11	6	0.2
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD12	6	0.2
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD13	6	0.2
(1,39)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	6	0.2
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG2	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:3:A:GLU:H	1:3:A:GLU:HG3	10	0.2
(4,62)	1:5:A:VAL:HG11	1:9:A:ILE:H	3	0.19
(4,62)	1:5:A:VAL:HG12	1:9:A:ILE:H	3	0.19
(4,62)	1:5:A:VAL:HG13	1:9:A:ILE:H	3	0.19
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD2	10	0.19
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD3	10	0.19
(4,38)	1:3:A:GLU:H	1:5:A:VAL:HB	1	0.19
(4,38)	1:3:A:GLU:H	1:5:A:VAL:HB	9	0.19
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	3	0.19
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	3	0.19
(4,23)	1:19:A:SER:HA	1:19:A:SER:HB3	5	0.19
(4,10)	1:9:A:ILE:H	1:9:A:ILE:HG12	2	0.19
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD11	7	0.19
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD12	7	0.19
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD13	7	0.19
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.19
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.19
(4,8)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.19
(3,602)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	4	0.19
(3,597)	1:16:A:GLY:H	1:17:A:PRO:HD2	2	0.19
(3,591)	1:2:A:GLU:HG3	1:4:A:ALA:H	4	0.19
(3,585)	1:5:A:VAL:HG11	1:6:A:ARG:HG3	6	0.19
(3,585)	1:5:A:VAL:HG12	1:6:A:ARG:HG3	6	0.19
(3,585)	1:5:A:VAL:HG13	1:6:A:ARG:HG3	6	0.19
(3,480)	1:8:A:TYR:HA	1:24:A:PRO:HB3	4	0.19
(3,423)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	0.19
(3,423)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	0.19
(3,423)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	0.19
(3,407)	1:12:A:LEU:HD11	1:16:A:GLY:H	10	0.19
(3,407)	1:12:A:LEU:HD12	1:16:A:GLY:H	10	0.19
(3,407)	1:12:A:LEU:HD13	1:16:A:GLY:H	10	0.19
(3,357)	1:8:A:TYR:HD1	1:11:A:TRP:H	4	0.19
(3,357)	1:8:A:TYR:HD2	1:11:A:TRP:H	4	0.19
(3,357)	1:8:A:TYR:HD1	1:11:A:TRP:H	6	0.19
(3,357)	1:8:A:TYR:HD2	1:11:A:TRP:H	6	0.19
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE1	9	0.19
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE2	9	0.19
(3,224)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	9	0.19
(3,44)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.19
(2,1)	1:8:A:TYR:HE1	1:24:A:PRO:HG2	4	0.19
(2,1)	1:8:A:TYR:HE2	1:24:A:PRO:HG2	4	0.19
(1,673)	1:8:A:TYR:HB3	1:24:A:PRO:HB2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,664)	1:16:A:GLY:H	1:17:A:PRO:HD2	2	0.19
(1,658)	1:2:A:GLU:HG3	1:4:A:ALA:H	4	0.19
(1,649)	1:5:A:VAL:HG11	1:6:A:ARG:HG3	6	0.19
(1,649)	1:5:A:VAL:HG12	1:6:A:ARG:HG3	6	0.19
(1,649)	1:5:A:VAL:HG13	1:6:A:ARG:HG3	6	0.19
(1,613)	1:5:A:VAL:HG11	1:9:A:ILE:H	3	0.19
(1,613)	1:5:A:VAL:HG12	1:9:A:ILE:H	3	0.19
(1,613)	1:5:A:VAL:HG13	1:9:A:ILE:H	3	0.19
(1,532)	1:8:A:TYR:HA	1:24:A:PRO:HB3	4	0.19
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD2	10	0.19
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD3	10	0.19
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	0.19
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	0.19
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	0.19
(1,449)	1:12:A:LEU:HD11	1:16:A:GLY:H	10	0.19
(1,449)	1:12:A:LEU:HD12	1:16:A:GLY:H	10	0.19
(1,449)	1:12:A:LEU:HD13	1:16:A:GLY:H	10	0.19
(1,417)	1:3:A:GLU:H	1:5:A:VAL:HB	1	0.19
(1,417)	1:3:A:GLU:H	1:5:A:VAL:HB	9	0.19
(1,391)	1:8:A:TYR:HD1	1:11:A:TRP:H	4	0.19
(1,391)	1:8:A:TYR:HD2	1:11:A:TRP:H	4	0.19
(1,391)	1:8:A:TYR:HD1	1:11:A:TRP:H	6	0.19
(1,391)	1:8:A:TYR:HD2	1:11:A:TRP:H	6	0.19
(1,391)	1:8:A:TYR:HD1	1:11:A:TRP:H	8	0.19
(1,391)	1:8:A:TYR:HD2	1:11:A:TRP:H	8	0.19
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE1	9	0.19
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE2	9	0.19
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	3	0.19
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	3	0.19
(1,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	9	0.19
(1,205)	1:19:A:SER:HA	1:19:A:SER:HB3	5	0.19
(1,68)	1:9:A:ILE:H	1:9:A:ILE:HG12	2	0.19
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD11	7	0.19
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD12	7	0.19
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD13	7	0.19
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.19
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.19
(1,59)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.19
(1,51)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.19
(4,69)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	4	0.18
(4,69)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	4	0.18
(4,34)	1:8:A:TYR:HD1	1:12:A:LEU:H	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:8:A:TYR:HD2	1:12:A:LEU:H	4	0.18
(4,34)	1:8:A:TYR:HD1	1:12:A:LEU:H	5	0.18
(4,34)	1:8:A:TYR:HD2	1:12:A:LEU:H	5	0.18
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	10	0.18
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	10	0.18
(4,23)	1:19:A:SER:HA	1:19:A:SER:HB3	2	0.18
(4,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	8	0.18
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	3	0.18
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	3	0.18
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	3	0.18
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	3	0.18
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	3	0.18
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	3	0.18
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	3	0.18
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	3	0.18
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	3	0.18
(3,591)	1:2:A:GLU:HG3	1:4:A:ALA:H	3	0.18
(3,568)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	9	0.18
(3,561)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	6	0.18
(3,561)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	8	0.18
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	4	0.18
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	4	0.18
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	4	0.18
(3,528)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	3	0.18
(3,528)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	3	0.18
(3,528)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	3	0.18
(3,528)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	10	0.18
(3,528)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	10	0.18
(3,528)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	10	0.18
(3,491)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	8	0.18
(3,480)	1:8:A:TYR:HA	1:24:A:PRO:HB3	6	0.18
(3,480)	1:8:A:TYR:HA	1:24:A:PRO:HB3	10	0.18
(3,439)	1:10:A:GLN:H	1:11:A:TRP:HB2	4	0.18
(3,429)	1:11:A:TRP:H	1:24:A:PRO:HG2	6	0.18
(3,423)	1:5:A:VAL:HG21	1:6:A:ARG:H	7	0.18
(3,423)	1:5:A:VAL:HG22	1:6:A:ARG:H	7	0.18
(3,423)	1:5:A:VAL:HG23	1:6:A:ARG:H	7	0.18
(3,357)	1:8:A:TYR:HD1	1:11:A:TRP:H	1	0.18
(3,357)	1:8:A:TYR:HD2	1:11:A:TRP:H	1	0.18
(3,357)	1:8:A:TYR:HD1	1:11:A:TRP:H	5	0.18
(3,357)	1:8:A:TYR:HD2	1:11:A:TRP:H	5	0.18
(3,357)	1:8:A:TYR:HD1	1:11:A:TRP:H	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,357)	1:8:A:TYR:HD2	1:11:A:TRP:H	8	0.18
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE1	3	0.18
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE2	3	0.18
(3,224)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	1	0.18
(3,224)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	2	0.18
(3,224)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	3	0.18
(3,224)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	6	0.18
(3,164)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	2	0.18
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	3	0.18
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	3	0.18
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	3	0.18
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	3	0.18
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	3	0.18
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	3	0.18
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	3	0.18
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	3	0.18
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	3	0.18
(1,669)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	4	0.18
(1,669)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	4	0.18
(1,658)	1:2:A:GLU:HG3	1:4:A:ALA:H	3	0.18
(1,631)	1:11:A:TRP:HD1	1:21:A:ARG:HD3	9	0.18
(1,624)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	6	0.18
(1,624)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	8	0.18
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	4	0.18
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	4	0.18
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	4	0.18
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	5	0.18
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	5	0.18
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	5	0.18
(1,585)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	3	0.18
(1,585)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	3	0.18
(1,585)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	3	0.18
(1,585)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	10	0.18
(1,585)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	10	0.18
(1,585)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	10	0.18
(1,545)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	8	0.18
(1,532)	1:8:A:TYR:HA	1:24:A:PRO:HB3	6	0.18
(1,532)	1:8:A:TYR:HA	1:24:A:PRO:HB3	10	0.18
(1,488)	1:10:A:GLN:H	1:11:A:TRP:HB2	4	0.18
(1,476)	1:11:A:TRP:H	1:24:A:PRO:HG2	6	0.18
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:H	7	0.18
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:H	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:H	7	0.18
(1,391)	1:8:A:TYR:HD1	1:11:A:TRP:H	1	0.18
(1,391)	1:8:A:TYR:HD2	1:11:A:TRP:H	1	0.18
(1,391)	1:8:A:TYR:HD1	1:11:A:TRP:H	5	0.18
(1,391)	1:8:A:TYR:HD2	1:11:A:TRP:H	5	0.18
(1,389)	1:8:A:TYR:HD1	1:12:A:LEU:H	4	0.18
(1,389)	1:8:A:TYR:HD2	1:12:A:LEU:H	4	0.18
(1,389)	1:8:A:TYR:HD1	1:12:A:LEU:H	5	0.18
(1,389)	1:8:A:TYR:HD2	1:12:A:LEU:H	5	0.18
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE1	3	0.18
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE2	3	0.18
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	10	0.18
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	10	0.18
(1,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	1	0.18
(1,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	2	0.18
(1,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	3	0.18
(1,247)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	6	0.18
(1,205)	1:19:A:SER:HA	1:19:A:SER:HB3	2	0.18
(1,186)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	2	0.18
(1,35)	1:6:A:ARG:HA	1:6:A:ARG:HG2	8	0.18
(4,69)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	5	0.17
(4,69)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	5	0.17
(4,69)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	7	0.17
(4,69)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	7	0.17
(4,53)	1:3:A:GLU:HA	1:6:A:ARG:HB2	2	0.17
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD2	8	0.17
(4,47)	1:10:A:GLN:H	1:13:A:LYS:HD3	8	0.17
(4,38)	1:3:A:GLU:H	1:5:A:VAL:HB	7	0.17
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	9	0.17
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	9	0.17
(4,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	5	0.17
(4,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	7	0.17
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG21	1	0.17
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG22	1	0.17
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG23	1	0.17
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG21	7	0.17
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG22	7	0.17
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG23	7	0.17
(3,551)	1:10:A:GLN:H	1:10:A:GLN:HE21	2	0.17
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	5	0.17
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	5	0.17
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	10	0.17
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	10	0.17
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	10	0.17
(3,491)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	6	0.17
(3,491)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	9	0.17
(3,480)	1:8:A:TYR:HA	1:24:A:PRO:HB3	9	0.17
(3,437)	1:10:A:GLN:HG2	1:11:A:TRP:H	4	0.17
(3,429)	1:11:A:TRP:H	1:24:A:PRO:HG2	3	0.17
(3,429)	1:11:A:TRP:H	1:24:A:PRO:HG2	10	0.17
(3,417)	1:8:A:TYR:H	1:24:A:PRO:HB3	9	0.17
(3,417)	1:8:A:TYR:H	1:24:A:PRO:HB3	10	0.17
(3,357)	1:8:A:TYR:HD1	1:11:A:TRP:H	9	0.17
(3,357)	1:8:A:TYR:HD2	1:11:A:TRP:H	9	0.17
(3,289)	1:8:A:TYR:HD1	1:9:A:ILE:HB	3	0.17
(3,289)	1:8:A:TYR:HD2	1:9:A:ILE:HB	3	0.17
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE1	6	0.17
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE2	6	0.17
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE1	10	0.17
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE2	10	0.17
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG21	1	0.17
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG22	1	0.17
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG23	1	0.17
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG21	7	0.17
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG22	7	0.17
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG23	7	0.17
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	6	0.17
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	6	0.17
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	6	0.17
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	6	0.17
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	6	0.17
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	6	0.17
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	6	0.17
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	6	0.17
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	6	0.17
(1,669)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	5	0.17
(1,669)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	5	0.17
(1,669)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	7	0.17
(1,669)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	7	0.17
(1,612)	1:10:A:GLN:H	1:10:A:GLN:HE21	2	0.17
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	10	0.17
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	10	0.17
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,545)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	6	0.17
(1,545)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	9	0.17
(1,534)	1:3:A:GLU:HA	1:6:A:ARG:HB2	2	0.17
(1,532)	1:8:A:TYR:HA	1:24:A:PRO:HB3	9	0.17
(1,486)	1:10:A:GLN:HG2	1:11:A:TRP:H	4	0.17
(1,476)	1:11:A:TRP:H	1:24:A:PRO:HG2	3	0.17
(1,476)	1:11:A:TRP:H	1:24:A:PRO:HG2	10	0.17
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD2	8	0.17
(1,473)	1:10:A:GLN:H	1:13:A:LYS:HD3	8	0.17
(1,459)	1:8:A:TYR:H	1:24:A:PRO:HB3	9	0.17
(1,459)	1:8:A:TYR:H	1:24:A:PRO:HB3	10	0.17
(1,417)	1:3:A:GLU:H	1:5:A:VAL:HB	7	0.17
(1,391)	1:8:A:TYR:HD1	1:11:A:TRP:H	9	0.17
(1,391)	1:8:A:TYR:HD2	1:11:A:TRP:H	9	0.17
(1,317)	1:8:A:TYR:HD1	1:9:A:ILE:HB	3	0.17
(1,317)	1:8:A:TYR:HD2	1:9:A:ILE:HB	3	0.17
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE1	6	0.17
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE2	6	0.17
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE1	10	0.17
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE2	10	0.17
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	9	0.17
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	9	0.17
(1,35)	1:6:A:ARG:HA	1:6:A:ARG:HG2	5	0.17
(1,35)	1:6:A:ARG:HA	1:6:A:ARG:HG2	7	0.17
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	6	0.16
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	6	0.16
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	6	0.16
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	6	0.16
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	6	0.16
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	6	0.16
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	6	0.16
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	6	0.16
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	6	0.16
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	10	0.16
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	10	0.16
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	10	0.16
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	10	0.16
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	10	0.16
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	10	0.16
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	10	0.16
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	10	0.16
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,583)	1:2:A:GLU:HG3	1:5:A:VAL:HB	6	0.16
(3,583)	1:2:A:GLU:HG3	1:5:A:VAL:HB	8	0.16
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	6	0.16
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	6	0.16
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	6	0.16
(3,491)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	7	0.16
(3,439)	1:10:A:GLN:H	1:11:A:TRP:HB2	2	0.16
(3,429)	1:11:A:TRP:H	1:24:A:PRO:HG2	5	0.16
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE1	4	0.16
(3,271)	1:8:A:TYR:HA	1:8:A:TYR:HE2	4	0.16
(3,211)	1:21:A:ARG:HA	1:22:A:PRO:HD2	9	0.16
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	1	0.16
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	1	0.16
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	2	0.16
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	2	0.16
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	3	0.16
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	3	0.16
(3,138)	1:13:A:LYS:H	1:13:A:LYS:HD2	10	0.16
(3,128)	1:13:A:LYS:HA	1:13:A:LYS:HG3	7	0.16
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	10	0.16
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	10	0.16
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	10	0.16
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	10	0.16
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	10	0.16
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	10	0.16
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	10	0.16
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	10	0.16
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	10	0.16
(1,646)	1:2:A:GLU:HG3	1:5:A:VAL:HB	6	0.16
(1,646)	1:2:A:GLU:HG3	1:5:A:VAL:HB	8	0.16
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	6	0.16
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	6	0.16
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	6	0.16
(1,545)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	7	0.16
(1,488)	1:10:A:GLN:H	1:11:A:TRP:HB2	2	0.16
(1,476)	1:11:A:TRP:H	1:24:A:PRO:HG2	5	0.16
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE1	4	0.16
(1,297)	1:8:A:TYR:HA	1:8:A:TYR:HE2	4	0.16
(1,234)	1:21:A:ARG:HA	1:22:A:PRO:HD2	9	0.16
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	1	0.16
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	1	0.16
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	2	0.16
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	3	0.16
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	3	0.16
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	9	0.16
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	9	0.16
(1,159)	1:13:A:LYS:H	1:13:A:LYS:HD2	10	0.16
(1,149)	1:13:A:LYS:HA	1:13:A:LYS:HG3	7	0.16
(4,69)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	8	0.15
(4,69)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	8	0.15
(4,34)	1:8:A:TYR:HD1	1:12:A:LEU:H	7	0.15
(4,34)	1:8:A:TYR:HD2	1:12:A:LEU:H	7	0.15
(4,34)	1:8:A:TYR:HD1	1:12:A:LEU:H	8	0.15
(4,34)	1:8:A:TYR:HD2	1:12:A:LEU:H	8	0.15
(4,34)	1:8:A:TYR:HD1	1:12:A:LEU:H	9	0.15
(4,34)	1:8:A:TYR:HD2	1:12:A:LEU:H	9	0.15
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	8	0.15
(4,26)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	8	0.15
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD21	6	0.15
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD22	6	0.15
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD23	6	0.15
(4,10)	1:9:A:ILE:H	1:9:A:ILE:HG12	9	0.15
(3,583)	1:2:A:GLU:HG3	1:5:A:VAL:HB	5	0.15
(3,583)	1:2:A:GLU:HG3	1:5:A:VAL:HB	9	0.15
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	8	0.15
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	8	0.15
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	8	0.15
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	8	0.15
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	8	0.15
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	8	0.15
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	10	0.15
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	10	0.15
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	10	0.15
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	10	0.15
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	10	0.15
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	10	0.15
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	2	0.15
(3,498)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	2	0.15
(3,491)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	10	0.15
(3,439)	1:10:A:GLN:H	1:11:A:TRP:HB2	3	0.15
(3,439)	1:10:A:GLN:H	1:11:A:TRP:HB2	6	0.15
(3,437)	1:10:A:GLN:HG2	1:11:A:TRP:H	3	0.15
(3,429)	1:11:A:TRP:H	1:24:A:PRO:HG2	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,429)	1:11:A:TRP:H	1:24:A:PRO:HG2	2	0.15
(3,417)	1:8:A:TYR:H	1:24:A:PRO:HB3	3	0.15
(3,357)	1:8:A:TYR:HD1	1:11:A:TRP:H	10	0.15
(3,357)	1:8:A:TYR:HD2	1:11:A:TRP:H	10	0.15
(3,293)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	3	0.15
(3,293)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	3	0.15
(3,293)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	10	0.15
(3,293)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	10	0.15
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	6	0.15
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	6	0.15
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	9	0.15
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	9	0.15
(3,164)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	1	0.15
(3,164)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	3	0.15
(3,164)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	4	0.15
(3,164)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	9	0.15
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	2	0.15
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	2	0.15
(3,132)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	2	0.15
(3,128)	1:13:A:LYS:HA	1:13:A:LYS:HG3	4	0.15
(1,669)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	8	0.15
(1,669)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	8	0.15
(1,646)	1:2:A:GLU:HG3	1:5:A:VAL:HB	5	0.15
(1,646)	1:2:A:GLU:HG3	1:5:A:VAL:HB	9	0.15
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	8	0.15
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	8	0.15
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	8	0.15
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	8	0.15
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	8	0.15
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	8	0.15
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	10	0.15
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	10	0.15
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	10	0.15
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	10	0.15
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	10	0.15
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	10	0.15
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG2	2	0.15
(1,552)	1:16:A:GLY:HA2	1:17:A:PRO:HG3	2	0.15
(1,545)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	10	0.15
(1,488)	1:10:A:GLN:H	1:11:A:TRP:HB2	3	0.15
(1,488)	1:10:A:GLN:H	1:11:A:TRP:HB2	6	0.15
(1,486)	1:10:A:GLN:HG2	1:11:A:TRP:H	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,476)	1:11:A:TRP:H	1:24:A:PRO:HG2	1	0.15
(1,476)	1:11:A:TRP:H	1:24:A:PRO:HG2	2	0.15
(1,459)	1:8:A:TYR:H	1:24:A:PRO:HB3	3	0.15
(1,391)	1:8:A:TYR:HD1	1:11:A:TRP:H	10	0.15
(1,391)	1:8:A:TYR:HD2	1:11:A:TRP:H	10	0.15
(1,389)	1:8:A:TYR:HD1	1:12:A:LEU:H	7	0.15
(1,389)	1:8:A:TYR:HD2	1:12:A:LEU:H	7	0.15
(1,389)	1:8:A:TYR:HD1	1:12:A:LEU:H	8	0.15
(1,389)	1:8:A:TYR:HD2	1:12:A:LEU:H	8	0.15
(1,389)	1:8:A:TYR:HD1	1:12:A:LEU:H	9	0.15
(1,389)	1:8:A:TYR:HD2	1:12:A:LEU:H	9	0.15
(1,322)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	3	0.15
(1,322)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	3	0.15
(1,322)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	10	0.15
(1,322)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	10	0.15
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD2	8	0.15
(1,294)	1:10:A:GLN:HE22	1:13:A:LYS:HD3	8	0.15
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	6	0.15
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	6	0.15
(1,186)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	1	0.15
(1,186)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	3	0.15
(1,186)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	4	0.15
(1,186)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	9	0.15
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	2	0.15
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	2	0.15
(1,153)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	2	0.15
(1,149)	1:13:A:LYS:HA	1:13:A:LYS:HG3	4	0.15
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD21	6	0.15
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD22	6	0.15
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD23	6	0.15
(1,68)	1:9:A:ILE:H	1:9:A:ILE:HG12	9	0.15
(4,69)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	1	0.14
(4,69)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	1	0.14
(4,69)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	2	0.14
(4,69)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	2	0.14
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD21	7	0.14
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD22	7	0.14
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD23	7	0.14
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD21	8	0.14
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD22	8	0.14
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD23	8	0.14
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG21	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG22	2	0.14
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG23	2	0.14
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG21	10	0.14
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG22	10	0.14
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG23	10	0.14
(3,585)	1:5:A:VAL:HG11	1:6:A:ARG:HG3	3	0.14
(3,585)	1:5:A:VAL:HG12	1:6:A:ARG:HG3	3	0.14
(3,585)	1:5:A:VAL:HG13	1:6:A:ARG:HG3	3	0.14
(3,583)	1:2:A:GLU:HG3	1:5:A:VAL:HB	1	0.14
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	5	0.14
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	5	0.14
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	5	0.14
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	5	0.14
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	5	0.14
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	5	0.14
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	2	0.14
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	2	0.14
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	2	0.14
(3,515)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	2	0.14
(3,499)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	8	0.14
(3,437)	1:10:A:GLN:HG2	1:11:A:TRP:H	1	0.14
(3,429)	1:11:A:TRP:H	1:24:A:PRO:HG2	8	0.14
(3,417)	1:8:A:TYR:H	1:24:A:PRO:HB3	6	0.14
(3,407)	1:12:A:LEU:HD11	1:16:A:GLY:H	2	0.14
(3,407)	1:12:A:LEU:HD12	1:16:A:GLY:H	2	0.14
(3,407)	1:12:A:LEU:HD13	1:16:A:GLY:H	2	0.14
(3,357)	1:8:A:TYR:HD1	1:11:A:TRP:H	2	0.14
(3,357)	1:8:A:TYR:HD2	1:11:A:TRP:H	2	0.14
(3,344)	1:21:A:ARG:HD3	1:21:A:ARG:HH11	6	0.14
(3,344)	1:21:A:ARG:HD3	1:21:A:ARG:HH12	6	0.14
(3,289)	1:8:A:TYR:HD1	1:9:A:ILE:HB	8	0.14
(3,289)	1:8:A:TYR:HD2	1:9:A:ILE:HB	8	0.14
(3,177)	1:19:A:SER:H	1:19:A:SER:HB2	8	0.14
(3,177)	1:19:A:SER:H	1:19:A:SER:HB2	9	0.14
(3,164)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	5	0.14
(3,164)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	6	0.14
(3,164)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	7	0.14
(3,164)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	10	0.14
(3,152)	1:15:A:GLY:HA3	1:16:A:GLY:H	2	0.14
(3,138)	1:13:A:LYS:H	1:13:A:LYS:HD2	3	0.14
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	1	0.14
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,132)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	1	0.14
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	6	0.14
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	6	0.14
(3,132)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	6	0.14
(3,128)	1:13:A:LYS:HA	1:13:A:LYS:HG3	5	0.14
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG21	2	0.14
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG22	2	0.14
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG23	2	0.14
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG21	10	0.14
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG22	10	0.14
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG23	10	0.14
(1,669)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	1	0.14
(1,669)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	1	0.14
(1,669)	1:8:A:TYR:HE1	1:9:A:ILE:HG13	2	0.14
(1,669)	1:8:A:TYR:HE2	1:9:A:ILE:HG13	2	0.14
(1,649)	1:5:A:VAL:HG11	1:6:A:ARG:HG3	3	0.14
(1,649)	1:5:A:VAL:HG12	1:6:A:ARG:HG3	3	0.14
(1,649)	1:5:A:VAL:HG13	1:6:A:ARG:HG3	3	0.14
(1,646)	1:2:A:GLU:HG3	1:5:A:VAL:HB	1	0.14
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	5	0.14
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	5	0.14
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	5	0.14
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	5	0.14
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	5	0.14
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	5	0.14
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	2	0.14
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	2	0.14
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	2	0.14
(1,572)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	2	0.14
(1,553)	1:23:A:PRO:HB3	1:24:A:PRO:HD3	8	0.14
(1,488)	1:10:A:GLN:H	1:11:A:TRP:HB2	9	0.14
(1,486)	1:10:A:GLN:HG2	1:11:A:TRP:H	1	0.14
(1,476)	1:11:A:TRP:H	1:24:A:PRO:HG2	8	0.14
(1,459)	1:8:A:TYR:H	1:24:A:PRO:HB3	6	0.14
(1,449)	1:12:A:LEU:HD11	1:16:A:GLY:H	2	0.14
(1,449)	1:12:A:LEU:HD12	1:16:A:GLY:H	2	0.14
(1,449)	1:12:A:LEU:HD13	1:16:A:GLY:H	2	0.14
(1,391)	1:8:A:TYR:HD1	1:11:A:TRP:H	2	0.14
(1,391)	1:8:A:TYR:HD2	1:11:A:TRP:H	2	0.14
(1,375)	1:21:A:ARG:HD3	1:21:A:ARG:HH11	6	0.14
(1,375)	1:21:A:ARG:HD3	1:21:A:ARG:HH12	6	0.14
(1,317)	1:8:A:TYR:HD1	1:9:A:ILE:HB	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	1:8:A:TYR:HD2	1:9:A:ILE:HB	8	0.14
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	8	0.14
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	9	0.14
(1,186)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	5	0.14
(1,186)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	6	0.14
(1,186)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	7	0.14
(1,186)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	8	0.14
(1,186)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	10	0.14
(1,174)	1:15:A:GLY:HA3	1:16:A:GLY:H	2	0.14
(1,159)	1:13:A:LYS:H	1:13:A:LYS:HD2	3	0.14
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	1	0.14
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	1	0.14
(1,153)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	1	0.14
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	6	0.14
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	6	0.14
(1,153)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	6	0.14
(1,149)	1:13:A:LYS:HA	1:13:A:LYS:HG3	5	0.14
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD21	7	0.14
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD22	7	0.14
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD23	7	0.14
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD21	8	0.14
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD22	8	0.14
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD23	8	0.14
(4,44)	1:7:A:LEU:HD11	1:8:A:TYR:H	2	0.13
(4,44)	1:7:A:LEU:HD12	1:8:A:TYR:H	2	0.13
(4,44)	1:7:A:LEU:HD13	1:8:A:TYR:H	2	0.13
(4,44)	1:7:A:LEU:HD11	1:8:A:TYR:H	6	0.13
(4,44)	1:7:A:LEU:HD12	1:8:A:TYR:H	6	0.13
(4,44)	1:7:A:LEU:HD13	1:8:A:TYR:H	6	0.13
(4,34)	1:8:A:TYR:HD1	1:12:A:LEU:H	1	0.13
(4,34)	1:8:A:TYR:HD2	1:12:A:LEU:H	1	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD21	1	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD22	1	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD23	1	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD21	4	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD22	4	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD23	4	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD21	5	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD22	5	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD23	5	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD21	9	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD22	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD23	9	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD21	10	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD22	10	0.13
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD23	10	0.13
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG21	3	0.13
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG22	3	0.13
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG23	3	0.13
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG21	4	0.13
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG22	4	0.13
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG23	4	0.13
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	4	0.13
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	4	0.13
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	4	0.13
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	4	0.13
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	4	0.13
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	4	0.13
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	4	0.13
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	4	0.13
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	4	0.13
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	9	0.13
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	9	0.13
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	9	0.13
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	9	0.13
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	9	0.13
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	9	0.13
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	9	0.13
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	9	0.13
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	9	0.13
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG21	6	0.13
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG22	6	0.13
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG23	6	0.13
(3,583)	1:2:A:GLU:HG3	1:5:A:VAL:HB	2	0.13
(3,583)	1:2:A:GLU:HG3	1:5:A:VAL:HB	7	0.13
(3,575)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	0.13
(3,561)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	7	0.13
(3,478)	1:8:A:TYR:HA	1:24:A:PRO:HG3	4	0.13
(3,475)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.13
(3,439)	1:10:A:GLN:H	1:11:A:TRP:HB2	1	0.13
(3,439)	1:10:A:GLN:H	1:11:A:TRP:HB2	5	0.13
(3,439)	1:10:A:GLN:H	1:11:A:TRP:HB2	8	0.13
(3,439)	1:10:A:GLN:H	1:11:A:TRP:HB2	9	0.13
(3,439)	1:10:A:GLN:H	1:11:A:TRP:HB2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,437)	1:10:A:GLN:HG2	1:11:A:TRP:H	7	0.13
(3,429)	1:11:A:TRP:H	1:24:A:PRO:HG2	7	0.13
(3,429)	1:11:A:TRP:H	1:24:A:PRO:HG2	9	0.13
(3,418)	1:8:A:TYR:H	1:9:A:ILE:HG13	6	0.13
(3,418)	1:8:A:TYR:H	1:9:A:ILE:HG13	9	0.13
(3,412)	1:18:A:SER:HB2	1:19:A:SER:H	10	0.13
(3,392)	1:9:A:ILE:H	1:10:A:GLN:HB3	10	0.13
(3,354)	1:10:A:GLN:H	1:10:A:GLN:HE22	3	0.13
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	10	0.13
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	10	0.13
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	10	0.13
(3,296)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	3	0.13
(3,296)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	3	0.13
(3,296)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	3	0.13
(3,296)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	3	0.13
(3,296)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	3	0.13
(3,296)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	3	0.13
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	10	0.13
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.13
(3,177)	1:19:A:SER:H	1:19:A:SER:HB2	1	0.13
(3,177)	1:19:A:SER:H	1:19:A:SER:HB2	2	0.13
(3,177)	1:19:A:SER:H	1:19:A:SER:HB2	4	0.13
(3,177)	1:19:A:SER:H	1:19:A:SER:HB2	5	0.13
(3,177)	1:19:A:SER:H	1:19:A:SER:HB2	6	0.13
(3,177)	1:19:A:SER:H	1:19:A:SER:HB2	7	0.13
(3,177)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.13
(3,164)	1:17:A:PRO:HB3	1:17:A:PRO:HD2	8	0.13
(3,137)	1:13:A:LYS:H	1:13:A:LYS:HB2	10	0.13
(3,137)	1:13:A:LYS:H	1:13:A:LYS:HB3	10	0.13
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	9	0.13
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	9	0.13
(3,132)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	9	0.13
(3,110)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	2	0.13
(3,108)	1:10:A:GLN:HA	1:10:A:GLN:HE21	2	0.13
(3,27)	1:6:A:ARG:HA	1:6:A:ARG:HD3	10	0.13
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG21	3	0.13
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG22	3	0.13
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG23	3	0.13
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG21	4	0.13
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG22	4	0.13
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG23	4	0.13
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	4	0.13
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	4	0.13
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	4	0.13
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	4	0.13
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	4	0.13
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	4	0.13
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	4	0.13
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	4	0.13
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	9	0.13
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	9	0.13
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	9	0.13
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	9	0.13
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	9	0.13
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	9	0.13
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	9	0.13
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	9	0.13
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	9	0.13
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG21	6	0.13
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG22	6	0.13
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG23	6	0.13
(1,646)	1:2:A:GLU:HG3	1:5:A:VAL:HB	2	0.13
(1,646)	1:2:A:GLU:HG3	1:5:A:VAL:HB	7	0.13
(1,638)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	0.13
(1,624)	1:11:A:TRP:HH2	1:23:A:PRO:HB2	7	0.13
(1,530)	1:8:A:TYR:HA	1:24:A:PRO:HG3	4	0.13
(1,525)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.13
(1,488)	1:10:A:GLN:H	1:11:A:TRP:HB2	1	0.13
(1,488)	1:10:A:GLN:H	1:11:A:TRP:HB2	5	0.13
(1,488)	1:10:A:GLN:H	1:11:A:TRP:HB2	8	0.13
(1,488)	1:10:A:GLN:H	1:11:A:TRP:HB2	10	0.13
(1,486)	1:10:A:GLN:HG2	1:11:A:TRP:H	7	0.13
(1,476)	1:11:A:TRP:H	1:24:A:PRO:HG2	7	0.13
(1,476)	1:11:A:TRP:H	1:24:A:PRO:HG2	9	0.13
(1,463)	1:7:A:LEU:HD11	1:8:A:TYR:H	2	0.13
(1,463)	1:7:A:LEU:HD12	1:8:A:TYR:H	2	0.13
(1,463)	1:7:A:LEU:HD13	1:8:A:TYR:H	2	0.13
(1,463)	1:7:A:LEU:HD11	1:8:A:TYR:H	6	0.13
(1,463)	1:7:A:LEU:HD12	1:8:A:TYR:H	6	0.13
(1,463)	1:7:A:LEU:HD13	1:8:A:TYR:H	6	0.13
(1,461)	1:8:A:TYR:H	1:9:A:ILE:HG13	6	0.13
(1,461)	1:8:A:TYR:H	1:9:A:ILE:HG13	9	0.13
(1,454)	1:18:A:SER:HB2	1:19:A:SER:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,431)	1:9:A:ILE:H	1:10:A:GLN:HB3	10	0.13
(1,389)	1:8:A:TYR:HD1	1:12:A:LEU:H	1	0.13
(1,389)	1:8:A:TYR:HD2	1:12:A:LEU:H	1	0.13
(1,387)	1:10:A:GLN:H	1:10:A:GLN:HE22	3	0.13
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	10	0.13
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	10	0.13
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	10	0.13
(1,325)	1:8:A:TYR:HD1	1:12:A:LEU:HD11	3	0.13
(1,325)	1:8:A:TYR:HD1	1:12:A:LEU:HD12	3	0.13
(1,325)	1:8:A:TYR:HD1	1:12:A:LEU:HD13	3	0.13
(1,325)	1:8:A:TYR:HD2	1:12:A:LEU:HD11	3	0.13
(1,325)	1:8:A:TYR:HD2	1:12:A:LEU:HD12	3	0.13
(1,325)	1:8:A:TYR:HD2	1:12:A:LEU:HD13	3	0.13
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	10	0.13
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.13
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	1	0.13
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	2	0.13
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	4	0.13
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	5	0.13
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	6	0.13
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	7	0.13
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.13
(1,158)	1:13:A:LYS:H	1:13:A:LYS:HB2	10	0.13
(1,158)	1:13:A:LYS:H	1:13:A:LYS:HB3	10	0.13
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	9	0.13
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	9	0.13
(1,153)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	9	0.13
(1,131)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	2	0.13
(1,129)	1:10:A:GLN:HA	1:10:A:GLN:HE21	2	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD21	1	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD22	1	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD23	1	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD21	4	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD22	4	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD23	4	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD21	5	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD22	5	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD23	5	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD21	9	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD22	9	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD23	9	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD21	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD22	10	0.13
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD23	10	0.13
(1,32)	1:6:A:ARG:HA	1:6:A:ARG:HD3	10	0.13
(4,52)	1:1:A:GLU:HB2	1:2:A:GLU:HA	4	0.12
(4,52)	1:1:A:GLU:HB2	1:2:A:GLU:HA	10	0.12
(4,44)	1:7:A:LEU:HD11	1:8:A:TYR:H	3	0.12
(4,44)	1:7:A:LEU:HD12	1:8:A:TYR:H	3	0.12
(4,44)	1:7:A:LEU:HD13	1:8:A:TYR:H	3	0.12
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD21	2	0.12
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD22	2	0.12
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD23	2	0.12
(4,7)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.12
(4,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	6	0.12
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG21	5	0.12
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG22	5	0.12
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG23	5	0.12
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG21	9	0.12
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG22	9	0.12
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG23	9	0.12
(3,605)	1:9:A:ILE:HG21	1:13:A:LYS:HG3	1	0.12
(3,605)	1:9:A:ILE:HG22	1:13:A:LYS:HG3	1	0.12
(3,605)	1:9:A:ILE:HG23	1:13:A:LYS:HG3	1	0.12
(3,605)	1:9:A:ILE:HG21	1:13:A:LYS:HG3	6	0.12
(3,605)	1:9:A:ILE:HG22	1:13:A:LYS:HG3	6	0.12
(3,605)	1:9:A:ILE:HG23	1:13:A:LYS:HG3	6	0.12
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	5	0.12
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	5	0.12
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	5	0.12
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	5	0.12
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	5	0.12
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	5	0.12
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	5	0.12
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	5	0.12
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	5	0.12
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	8	0.12
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	8	0.12
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	8	0.12
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	8	0.12
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	8	0.12
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	8	0.12
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	8	0.12
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	8	0.12
(3,595)	1:5:A:VAL:HA	1:8:A:TYR:H	6	0.12
(3,438)	1:10:A:GLN:H	1:11:A:TRP:HB3	3	0.12
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD11	6	0.12
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD12	6	0.12
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD13	6	0.12
(3,359)	1:8:A:TYR:HE1	1:11:A:TRP:HZ3	3	0.12
(3,359)	1:8:A:TYR:HE2	1:11:A:TRP:HZ3	3	0.12
(3,354)	1:10:A:GLN:H	1:10:A:GLN:HE22	8	0.12
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	6	0.12
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	6	0.12
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	6	0.12
(3,293)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	6	0.12
(3,293)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	6	0.12
(3,289)	1:8:A:TYR:HD1	1:9:A:ILE:HB	1	0.12
(3,289)	1:8:A:TYR:HD2	1:9:A:ILE:HB	1	0.12
(3,289)	1:8:A:TYR:HD1	1:9:A:ILE:HB	10	0.12
(3,289)	1:8:A:TYR:HD2	1:9:A:ILE:HB	10	0.12
(3,284)	1:11:A:TRP:HD1	1:23:A:PRO:HA	8	0.12
(3,211)	1:21:A:ARG:HA	1:22:A:PRO:HD2	1	0.12
(3,211)	1:21:A:ARG:HA	1:22:A:PRO:HD2	2	0.12
(3,138)	1:13:A:LYS:H	1:13:A:LYS:HD2	5	0.12
(3,137)	1:13:A:LYS:H	1:13:A:LYS:HB2	8	0.12
(3,137)	1:13:A:LYS:H	1:13:A:LYS:HB3	8	0.12
(3,128)	1:13:A:LYS:HA	1:13:A:LYS:HG3	1	0.12
(3,128)	1:13:A:LYS:HA	1:13:A:LYS:HG3	6	0.12
(3,11)	1:3:A:GLU:H	1:3:A:GLU:HB2	6	0.12
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG21	5	0.12
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG22	5	0.12
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG23	5	0.12
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG21	9	0.12
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG22	9	0.12
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG23	9	0.12
(1,677)	1:9:A:ILE:HG21	1:13:A:LYS:HG3	1	0.12
(1,677)	1:9:A:ILE:HG22	1:13:A:LYS:HG3	1	0.12
(1,677)	1:9:A:ILE:HG23	1:13:A:LYS:HG3	1	0.12
(1,677)	1:9:A:ILE:HG21	1:13:A:LYS:HG3	6	0.12
(1,677)	1:9:A:ILE:HG22	1:13:A:LYS:HG3	6	0.12
(1,677)	1:9:A:ILE:HG23	1:13:A:LYS:HG3	6	0.12
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	5	0.12
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	5	0.12
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	5	0.12
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	5	0.12
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	5	0.12
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	5	0.12
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	5	0.12
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	5	0.12
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	8	0.12
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	8	0.12
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	8	0.12
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	8	0.12
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	8	0.12
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	8	0.12
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	8	0.12
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	8	0.12
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	8	0.12
(1,662)	1:5:A:VAL:HA	1:8:A:TYR:H	6	0.12
(1,529)	1:1:A:GLU:HB2	1:2:A:GLU:HA	4	0.12
(1,529)	1:1:A:GLU:HB2	1:2:A:GLU:HA	10	0.12
(1,487)	1:10:A:GLN:H	1:11:A:TRP:HB3	3	0.12
(1,482)	1:10:A:GLN:HB2	1:11:A:TRP:H	10	0.12
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD11	6	0.12
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD12	6	0.12
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD13	6	0.12
(1,463)	1:7:A:LEU:HD11	1:8:A:TYR:H	3	0.12
(1,463)	1:7:A:LEU:HD12	1:8:A:TYR:H	3	0.12
(1,463)	1:7:A:LEU:HD13	1:8:A:TYR:H	3	0.12
(1,393)	1:8:A:TYR:HE1	1:11:A:TRP:HZ3	3	0.12
(1,393)	1:8:A:TYR:HE2	1:11:A:TRP:HZ3	3	0.12
(1,387)	1:10:A:GLN:H	1:10:A:GLN:HE22	8	0.12
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	6	0.12
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	6	0.12
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	6	0.12
(1,322)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	6	0.12
(1,322)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	6	0.12
(1,317)	1:8:A:TYR:HD1	1:9:A:ILE:HB	1	0.12
(1,317)	1:8:A:TYR:HD2	1:9:A:ILE:HB	1	0.12
(1,317)	1:8:A:TYR:HD1	1:9:A:ILE:HB	10	0.12
(1,317)	1:8:A:TYR:HD2	1:9:A:ILE:HB	10	0.12
(1,312)	1:11:A:TRP:HD1	1:23:A:PRO:HA	8	0.12
(1,234)	1:21:A:ARG:HA	1:22:A:PRO:HD2	1	0.12
(1,234)	1:21:A:ARG:HA	1:22:A:PRO:HD2	2	0.12
(1,159)	1:13:A:LYS:H	1:13:A:LYS:HD2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:13:A:LYS:H	1:13:A:LYS:HB2	8	0.12
(1,158)	1:13:A:LYS:H	1:13:A:LYS:HB3	8	0.12
(1,149)	1:13:A:LYS:HA	1:13:A:LYS:HG3	1	0.12
(1,149)	1:13:A:LYS:HA	1:13:A:LYS:HG3	6	0.12
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD21	2	0.12
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD22	2	0.12
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD23	2	0.12
(1,49)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.12
(1,35)	1:6:A:ARG:HA	1:6:A:ARG:HG2	6	0.12
(1,13)	1:3:A:GLU:H	1:3:A:GLU:HB2	6	0.12
(4,44)	1:7:A:LEU:HD11	1:8:A:TYR:H	10	0.11
(4,44)	1:7:A:LEU:HD12	1:8:A:TYR:H	10	0.11
(4,44)	1:7:A:LEU:HD13	1:8:A:TYR:H	10	0.11
(3,596)	1:10:A:GLN:HA	1:13:A:LYS:H	7	0.11
(3,596)	1:10:A:GLN:HA	1:13:A:LYS:H	8	0.11
(3,595)	1:5:A:VAL:HA	1:8:A:TYR:H	3	0.11
(3,593)	1:7:A:LEU:HD21	1:8:A:TYR:H	2	0.11
(3,593)	1:7:A:LEU:HD22	1:8:A:TYR:H	2	0.11
(3,593)	1:7:A:LEU:HD23	1:8:A:TYR:H	2	0.11
(3,593)	1:7:A:LEU:HD21	1:8:A:TYR:H	4	0.11
(3,593)	1:7:A:LEU:HD22	1:8:A:TYR:H	4	0.11
(3,593)	1:7:A:LEU:HD23	1:8:A:TYR:H	4	0.11
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG21	8	0.11
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG22	8	0.11
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG23	8	0.11
(3,585)	1:5:A:VAL:HG11	1:6:A:ARG:HG3	5	0.11
(3,585)	1:5:A:VAL:HG12	1:6:A:ARG:HG3	5	0.11
(3,585)	1:5:A:VAL:HG13	1:6:A:ARG:HG3	5	0.11
(3,549)	1:9:A:ILE:H	1:11:A:TRP:H	9	0.11
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	4	0.11
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	4	0.11
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	4	0.11
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	4	0.11
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	4	0.11
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	4	0.11
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	7	0.11
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	7	0.11
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	7	0.11
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	7	0.11
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	7	0.11
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	7	0.11
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	9	0.11
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	9	0.11
(3,533)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	9	0.11
(3,533)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	9	0.11
(3,533)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	9	0.11
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	7	0.11
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	7	0.11
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	7	0.11
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	8	0.11
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	8	0.11
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	8	0.11
(3,526)	1:5:A:VAL:HG21	1:9:A:ILE:HA	10	0.11
(3,526)	1:5:A:VAL:HG22	1:9:A:ILE:HA	10	0.11
(3,526)	1:5:A:VAL:HG23	1:9:A:ILE:HA	10	0.11
(3,511)	1:1:A:GLU:HG2	1:6:A:ARG:HG2	3	0.11
(3,511)	1:1:A:GLU:HG3	1:6:A:ARG:HG2	3	0.11
(3,439)	1:10:A:GLN:H	1:11:A:TRP:HB2	7	0.11
(3,438)	1:10:A:GLN:H	1:11:A:TRP:HB3	8	0.11
(3,437)	1:10:A:GLN:HG2	1:11:A:TRP:H	8	0.11
(3,435)	1:10:A:GLN:HB2	1:11:A:TRP:H	10	0.11
(3,423)	1:5:A:VAL:HG21	1:6:A:ARG:H	9	0.11
(3,423)	1:5:A:VAL:HG22	1:6:A:ARG:H	9	0.11
(3,423)	1:5:A:VAL:HG23	1:6:A:ARG:H	9	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD11	3	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD12	3	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD13	3	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD11	4	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD12	4	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD13	4	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD11	5	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD12	5	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD13	5	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD11	10	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD12	10	0.11
(3,420)	1:11:A:TRP:H	1:12:A:LEU:HD13	10	0.11
(3,418)	1:8:A:TYR:H	1:9:A:ILE:HG13	4	0.11
(3,418)	1:8:A:TYR:H	1:9:A:ILE:HG13	7	0.11
(3,418)	1:8:A:TYR:H	1:9:A:ILE:HG13	10	0.11
(3,392)	1:9:A:ILE:H	1:10:A:GLN:HB3	5	0.11
(3,354)	1:10:A:GLN:H	1:10:A:GLN:HE22	10	0.11
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	4	0.11
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	4	0.11
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	5	0.11
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	5	0.11
(3,337)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	5	0.11
(3,289)	1:8:A:TYR:HD1	1:9:A:ILE:HB	2	0.11
(3,289)	1:8:A:TYR:HD2	1:9:A:ILE:HB	2	0.11
(3,289)	1:8:A:TYR:HD1	1:9:A:ILE:HB	5	0.11
(3,289)	1:8:A:TYR:HD2	1:9:A:ILE:HB	5	0.11
(3,289)	1:8:A:TYR:HD1	1:9:A:ILE:HB	7	0.11
(3,289)	1:8:A:TYR:HD2	1:9:A:ILE:HB	7	0.11
(3,284)	1:11:A:TRP:HD1	1:23:A:PRO:HA	7	0.11
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	4	0.11
(3,201)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	4	0.11
(3,177)	1:19:A:SER:H	1:19:A:SER:HB2	3	0.11
(3,138)	1:13:A:LYS:H	1:13:A:LYS:HD2	8	0.11
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	8	0.11
(3,132)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	8	0.11
(3,132)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	8	0.11
(3,128)	1:13:A:LYS:HA	1:13:A:LYS:HG3	2	0.11
(3,111)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	10	0.11
(3,27)	1:6:A:ARG:HA	1:6:A:ARG:HD3	6	0.11
(1,663)	1:10:A:GLN:HA	1:13:A:LYS:H	7	0.11
(1,663)	1:10:A:GLN:HA	1:13:A:LYS:H	8	0.11
(1,662)	1:5:A:VAL:HA	1:8:A:TYR:H	2	0.11
(1,662)	1:5:A:VAL:HA	1:8:A:TYR:H	3	0.11
(1,660)	1:7:A:LEU:HD21	1:8:A:TYR:H	2	0.11
(1,660)	1:7:A:LEU:HD22	1:8:A:TYR:H	2	0.11
(1,660)	1:7:A:LEU:HD23	1:8:A:TYR:H	2	0.11
(1,660)	1:7:A:LEU:HD21	1:8:A:TYR:H	4	0.11
(1,660)	1:7:A:LEU:HD22	1:8:A:TYR:H	4	0.11
(1,660)	1:7:A:LEU:HD23	1:8:A:TYR:H	4	0.11
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG21	8	0.11
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG22	8	0.11
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG23	8	0.11
(1,649)	1:5:A:VAL:HG11	1:6:A:ARG:HG3	5	0.11
(1,649)	1:5:A:VAL:HG12	1:6:A:ARG:HG3	5	0.11
(1,649)	1:5:A:VAL:HG13	1:6:A:ARG:HG3	5	0.11
(1,610)	1:9:A:ILE:H	1:11:A:TRP:H	9	0.11
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	4	0.11
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	4	0.11
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	4	0.11
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	4	0.11
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	4	0.11
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	7	0.11
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	7	0.11
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	7	0.11
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	7	0.11
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	7	0.11
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	7	0.11
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	9	0.11
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	9	0.11
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	9	0.11
(1,590)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	9	0.11
(1,590)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	9	0.11
(1,590)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	9	0.11
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	7	0.11
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	7	0.11
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	7	0.11
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	8	0.11
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	8	0.11
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	8	0.11
(1,583)	1:5:A:VAL:HG21	1:9:A:ILE:HA	10	0.11
(1,583)	1:5:A:VAL:HG22	1:9:A:ILE:HA	10	0.11
(1,583)	1:5:A:VAL:HG23	1:9:A:ILE:HA	10	0.11
(1,568)	1:1:A:GLU:HG2	1:6:A:ARG:HG2	3	0.11
(1,568)	1:1:A:GLU:HG3	1:6:A:ARG:HG2	3	0.11
(1,488)	1:10:A:GLN:H	1:11:A:TRP:HB2	7	0.11
(1,487)	1:10:A:GLN:H	1:11:A:TRP:HB3	8	0.11
(1,486)	1:10:A:GLN:HG2	1:11:A:TRP:H	8	0.11
(1,468)	1:5:A:VAL:HG21	1:6:A:ARG:H	9	0.11
(1,468)	1:5:A:VAL:HG22	1:6:A:ARG:H	9	0.11
(1,468)	1:5:A:VAL:HG23	1:6:A:ARG:H	9	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD11	3	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD12	3	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD13	3	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD11	4	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD12	4	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD13	4	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD11	5	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD12	5	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD13	5	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD11	10	0.11
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD12	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,465)	1:11:A:TRP:H	1:12:A:LEU:HD13	10	0.11
(1,463)	1:7:A:LEU:HD11	1:8:A:TYR:H	10	0.11
(1,463)	1:7:A:LEU:HD12	1:8:A:TYR:H	10	0.11
(1,463)	1:7:A:LEU:HD13	1:8:A:TYR:H	10	0.11
(1,461)	1:8:A:TYR:H	1:9:A:ILE:HG13	4	0.11
(1,461)	1:8:A:TYR:H	1:9:A:ILE:HG13	7	0.11
(1,461)	1:8:A:TYR:H	1:9:A:ILE:HG13	10	0.11
(1,431)	1:9:A:ILE:H	1:10:A:GLN:HB3	5	0.11
(1,387)	1:10:A:GLN:H	1:10:A:GLN:HE22	10	0.11
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	4	0.11
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	4	0.11
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	4	0.11
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD11	5	0.11
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD12	5	0.11
(1,368)	1:11:A:TRP:HH2	1:12:A:LEU:HD13	5	0.11
(1,317)	1:8:A:TYR:HD1	1:9:A:ILE:HB	2	0.11
(1,317)	1:8:A:TYR:HD2	1:9:A:ILE:HB	2	0.11
(1,317)	1:8:A:TYR:HD1	1:9:A:ILE:HB	5	0.11
(1,317)	1:8:A:TYR:HD2	1:9:A:ILE:HB	5	0.11
(1,317)	1:8:A:TYR:HD1	1:9:A:ILE:HB	7	0.11
(1,317)	1:8:A:TYR:HD2	1:9:A:ILE:HB	7	0.11
(1,312)	1:11:A:TRP:HD1	1:23:A:PRO:HA	7	0.11
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	4	0.11
(1,224)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	4	0.11
(1,199)	1:19:A:SER:H	1:19:A:SER:HB2	3	0.11
(1,159)	1:13:A:LYS:H	1:13:A:LYS:HD2	8	0.11
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	8	0.11
(1,153)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	8	0.11
(1,153)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	8	0.11
(1,149)	1:13:A:LYS:HA	1:13:A:LYS:HG3	2	0.11
(1,132)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	10	0.11
(1,32)	1:6:A:ARG:HA	1:6:A:ARG:HD3	6	0.11
(4,52)	1:1:A:GLU:HB2	1:2:A:GLU:HA	3	0.1
(4,44)	1:7:A:LEU:HD11	1:8:A:TYR:H	4	0.1
(4,44)	1:7:A:LEU:HD12	1:8:A:TYR:H	4	0.1
(4,44)	1:7:A:LEU:HD13	1:8:A:TYR:H	4	0.1
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD21	3	0.1
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD22	3	0.1
(4,18)	1:7:A:LEU:H	1:7:A:LEU:HD23	3	0.1
(4,6)	1:6:A:ARG:HA	1:6:A:ARG:HG2	4	0.1
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG21	6	0.1
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG22	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG23	6	0.1
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG21	8	0.1
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG22	8	0.1
(3,609)	1:1:A:GLU:HA	1:5:A:VAL:HG23	8	0.1
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	7	0.1
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	7	0.1
(3,604)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	7	0.1
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	7	0.1
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	7	0.1
(3,604)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	7	0.1
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	7	0.1
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	7	0.1
(3,604)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	7	0.1
(3,595)	1:5:A:VAL:HA	1:8:A:TYR:H	2	0.1
(3,593)	1:7:A:LEU:HD21	1:8:A:TYR:H	3	0.1
(3,593)	1:7:A:LEU:HD22	1:8:A:TYR:H	3	0.1
(3,593)	1:7:A:LEU:HD23	1:8:A:TYR:H	3	0.1
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG21	5	0.1
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG22	5	0.1
(3,587)	1:1:A:GLU:HB3	1:5:A:VAL:HG23	5	0.1
(3,555)	1:2:A:GLU:HB2	1:4:A:ALA:H	6	0.1
(3,555)	1:2:A:GLU:HB3	1:4:A:ALA:H	6	0.1
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	1	0.1
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	1	0.1
(3,531)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	1	0.1
(3,508)	1:4:A:ALA:HB1	1:5:A:VAL:HB	3	0.1
(3,508)	1:4:A:ALA:HB2	1:5:A:VAL:HB	3	0.1
(3,508)	1:4:A:ALA:HB3	1:5:A:VAL:HB	3	0.1
(3,491)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	1	0.1
(3,418)	1:8:A:TYR:H	1:9:A:ILE:HG13	3	0.1
(3,298)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	3	0.1
(3,298)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	3	0.1
(3,298)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	3	0.1
(3,298)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	3	0.1
(3,298)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	3	0.1
(3,298)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	3	0.1
(3,289)	1:8:A:TYR:HD1	1:9:A:ILE:HB	4	0.1
(3,289)	1:8:A:TYR:HD2	1:9:A:ILE:HB	4	0.1
(3,137)	1:13:A:LYS:H	1:13:A:LYS:HB2	3	0.1
(3,137)	1:13:A:LYS:H	1:13:A:LYS:HB3	3	0.1
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG21	6	0.1
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG22	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG23	6	0.1
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG21	8	0.1
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG22	8	0.1
(1,682)	1:1:A:GLU:HA	1:5:A:VAL:HG23	8	0.1
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	7	0.1
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	7	0.1
(1,676)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	7	0.1
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	7	0.1
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	7	0.1
(1,676)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	7	0.1
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	7	0.1
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	7	0.1
(1,676)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	7	0.1
(1,660)	1:7:A:LEU:HD21	1:8:A:TYR:H	3	0.1
(1,660)	1:7:A:LEU:HD22	1:8:A:TYR:H	3	0.1
(1,660)	1:7:A:LEU:HD23	1:8:A:TYR:H	3	0.1
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG21	5	0.1
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG22	5	0.1
(1,652)	1:1:A:GLU:HB3	1:5:A:VAL:HG23	5	0.1
(1,617)	1:2:A:GLU:HB2	1:4:A:ALA:H	6	0.1
(1,617)	1:2:A:GLU:HB3	1:4:A:ALA:H	6	0.1
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD11	1	0.1
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD12	1	0.1
(1,588)	1:8:A:TYR:HB2	1:12:A:LEU:HD13	1	0.1
(1,564)	1:4:A:ALA:HB1	1:5:A:VAL:HB	3	0.1
(1,564)	1:4:A:ALA:HB2	1:5:A:VAL:HB	3	0.1
(1,564)	1:4:A:ALA:HB3	1:5:A:VAL:HB	3	0.1
(1,545)	1:14:A:ASP:HB2	1:15:A:GLY:HA3	1	0.1
(1,529)	1:1:A:GLU:HB2	1:2:A:GLU:HA	3	0.1
(1,463)	1:7:A:LEU:HD11	1:8:A:TYR:H	4	0.1
(1,463)	1:7:A:LEU:HD12	1:8:A:TYR:H	4	0.1
(1,463)	1:7:A:LEU:HD13	1:8:A:TYR:H	4	0.1
(1,461)	1:8:A:TYR:H	1:9:A:ILE:HG13	3	0.1
(1,327)	1:8:A:TYR:HD1	1:12:A:LEU:HD21	3	0.1
(1,327)	1:8:A:TYR:HD1	1:12:A:LEU:HD22	3	0.1
(1,327)	1:8:A:TYR:HD1	1:12:A:LEU:HD23	3	0.1
(1,327)	1:8:A:TYR:HD2	1:12:A:LEU:HD21	3	0.1
(1,327)	1:8:A:TYR:HD2	1:12:A:LEU:HD22	3	0.1
(1,327)	1:8:A:TYR:HD2	1:12:A:LEU:HD23	3	0.1
(1,317)	1:8:A:TYR:HD1	1:9:A:ILE:HB	4	0.1
(1,317)	1:8:A:TYR:HD2	1:9:A:ILE:HB	4	0.1
(1,158)	1:13:A:LYS:H	1:13:A:LYS:HB2	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:13:A:LYS:H	1:13:A:LYS:HB3	3	0.1
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD21	3	0.1
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD22	3	0.1
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HD23	3	0.1
(1,35)	1:6:A:ARG:HA	1:6:A:ARG:HG2	4	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found