



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 09:07 AM UTC

PDB ID : 5VFK / pdb_00005vfk
BMRB ID : 30279
Title : Solution structure of an archaeal DUF61 family protein SSO0941
Authors : Zhou, T.; Wang, J.; Feng, Y.
Deposited on : 2017-04-07

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

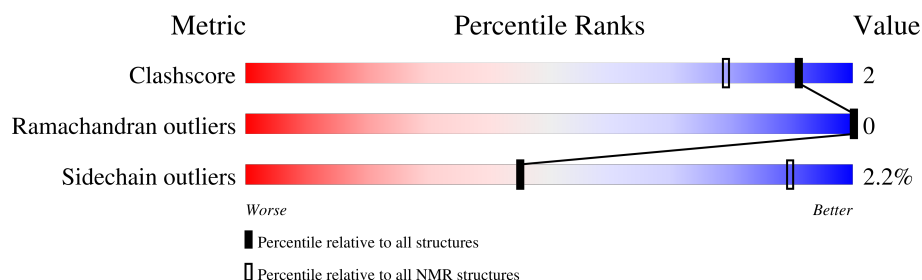
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 95%.

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	146	

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:17-A:73, A:77-A:122 (103)	0.35	18
2	A:130-A:138 (9)	0.27	11

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 5, 6, 7, 8, 10, 11, 12, 13, 14, 15, 17, 18, 19
2	9, 20
3	1, 16

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2448 atoms, of which 1238 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	146	Total	C	H	N	O	S	0
			2448	787	1238	197	224	2	

There are 8 discrepancies between the modelled and reference sequences:

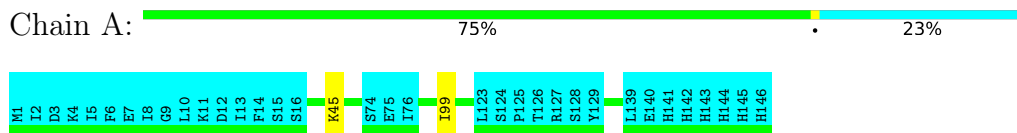
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	LEU	-	expression tag	UNP Q97ZH2
A	140	GLU	-	expression tag	UNP Q97ZH2
A	141	HIS	-	expression tag	UNP Q97ZH2
A	142	HIS	-	expression tag	UNP Q97ZH2
A	143	HIS	-	expression tag	UNP Q97ZH2
A	144	HIS	-	expression tag	UNP Q97ZH2
A	145	HIS	-	expression tag	UNP Q97ZH2
A	146	HIS	-	expression tag	UNP Q97ZH2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Uncharacterized protein

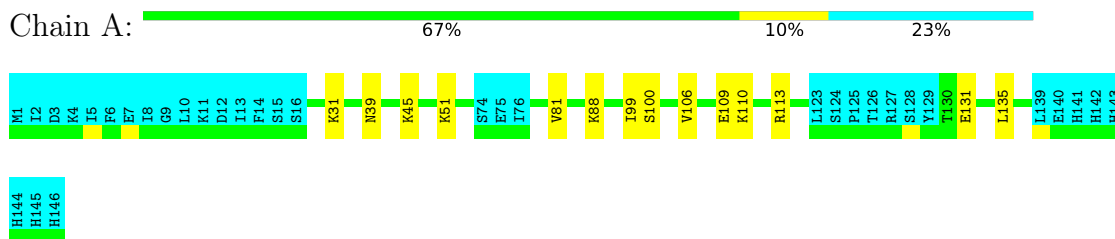


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

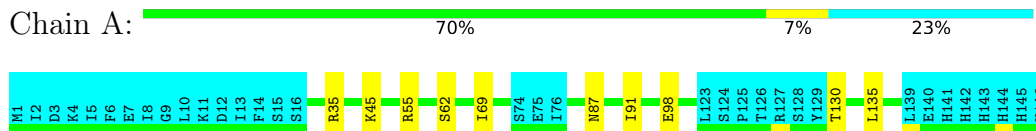
4.2.1 Score per residue for model 1

- Molecule 1: Uncharacterized protein



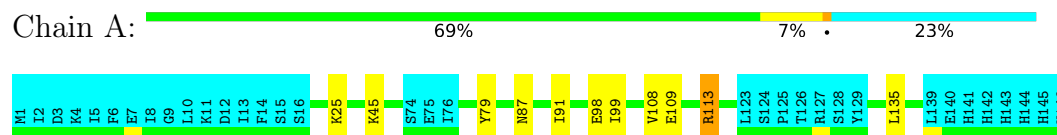
4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein



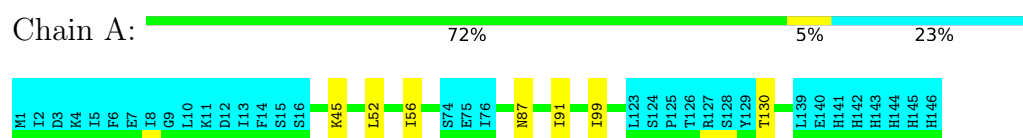
4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein



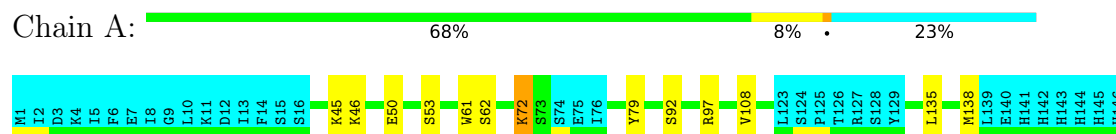
4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein



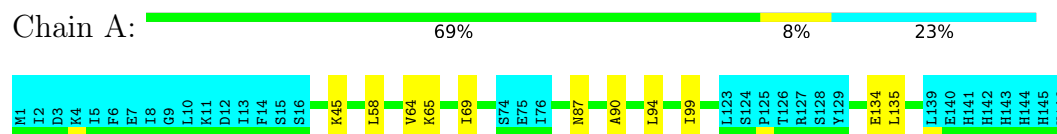
4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein



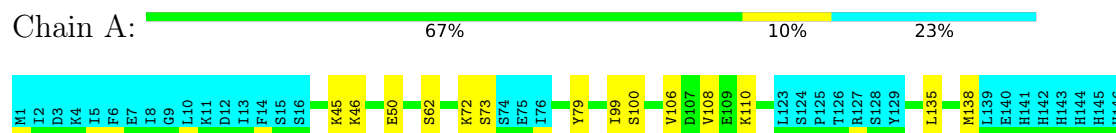
4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein



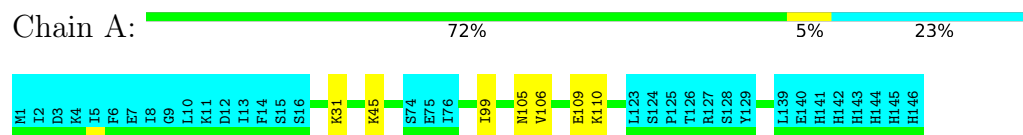
4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein



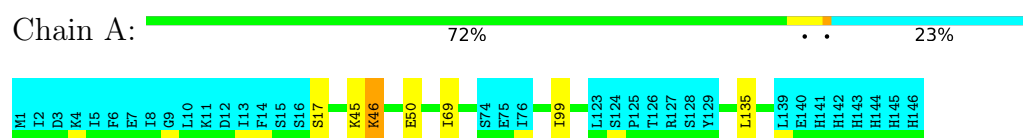
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein



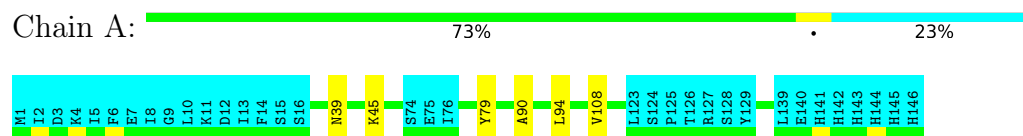
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein



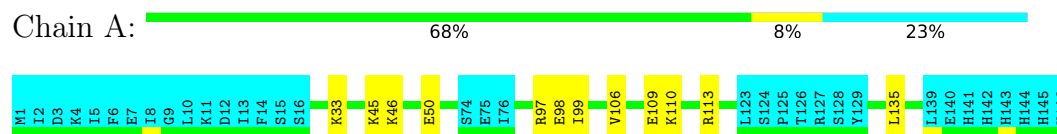
4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein



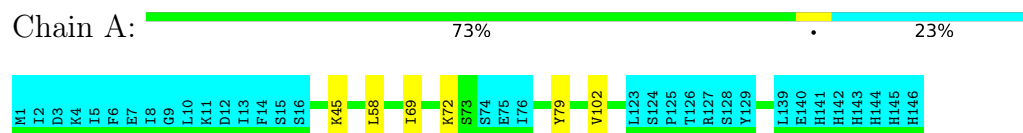
4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein



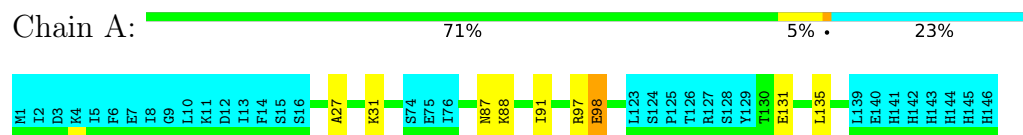
4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein



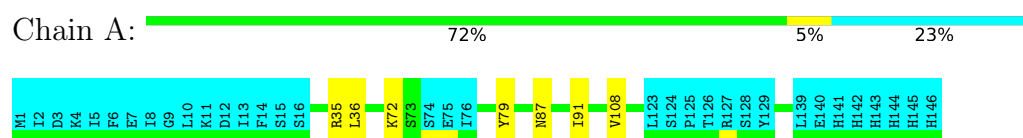
4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein



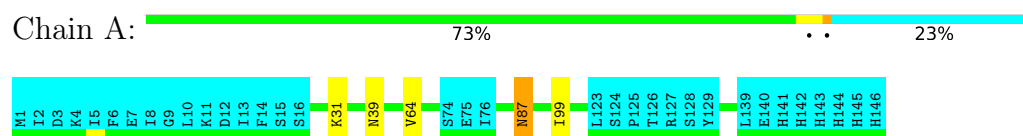
4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein



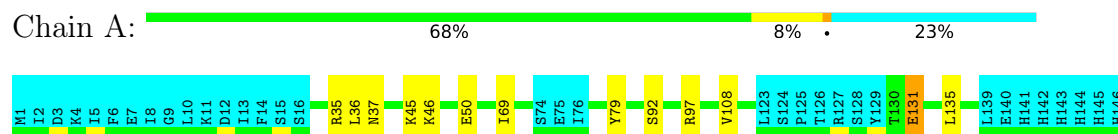
4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein



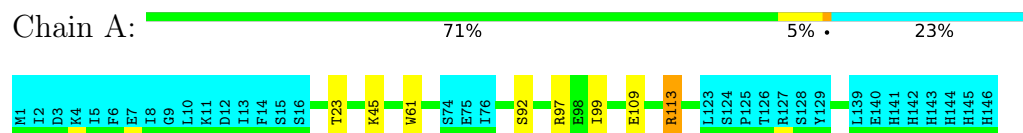
4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein



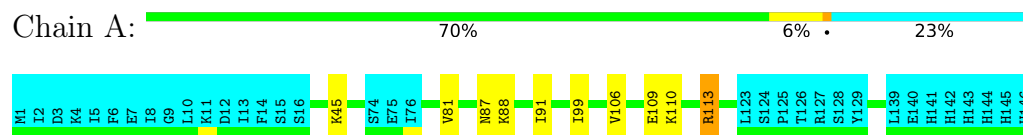
4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein



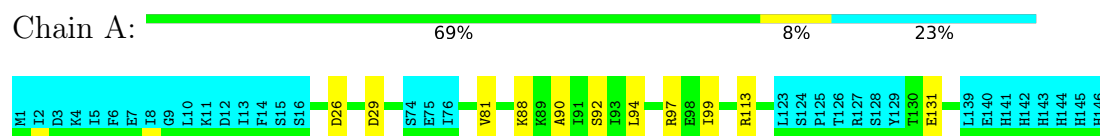
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Uncharacterized protein



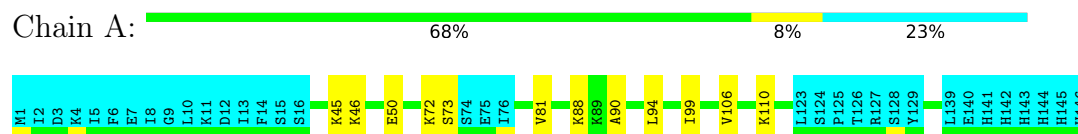
4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein



4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CYANA	structure calculation	
CNS	refinement	
SANE	refinement	

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	2014
Number of shifts mapped to atoms	1972
Number of unparsed shifts	0
Number of shifts with mapping errors	42
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	95%

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	1.04±0.02	1±1/941 (0.1± 0.1%)	0.97±0.02	0±0/1271 (0.0± 0.0%)
All	All	1.04	19/18820 (0.1%)	0.97	2/25420 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.3±0.6
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	99	ILE	CA-CB	5.50	1.60	1.54	9	13
1	A	69	ILE	CA-CB	5.49	1.61	1.54	9	5
1	A	31	LYS	C-N	-5.14	1.26	1.33	1	1

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	100	SER	N-CA-C	-5.74	103.77	112.04	7	1
1	A	102	VAL	N-CA-C	5.11	115.93	108.53	12	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	113	ARG	Sidechain	3
1	A	35	ARG	Sidechain	1
1	A	55	ARG	Sidechain	1
1	A	97	ARG	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	923	957	956	3±1
All	All	18460	19140	19120	62

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:GLU:O	1:A:113:ARG:HD3	0.57	1.99	11	3
1:A:135:LEU:O	1:A:138:MET:HG2	0.57	2.00	7	2
1:A:92:SER:HA	1:A:97:ARG:O	0.49	2.08	19	4
1:A:106:VAL:O	1:A:110:LYS:HG3	0.49	2.07	1	6
1:A:72:LYS:HD3	1:A:79:TYR:CZ	0.48	2.43	7	2
1:A:87:ASN:O	1:A:91:ILE:HG12	0.47	2.09	13	6
1:A:64:VAL:HA	1:A:87:ASN:ND2	0.47	2.25	15	2
1:A:90:ALA:O	1:A:94:LEU:HG	0.46	2.10	20	4
1:A:109:GLU:HB3	1:A:113:ARG:NH1	0.46	2.26	17	1
1:A:72:LYS:HG2	1:A:79:TYR:CE1	0.46	2.45	5	1
1:A:72:LYS:HG2	1:A:79:TYR:CE2	0.45	2.47	14	1
1:A:46:LYS:O	1:A:50:GLU:HG3	0.45	2.12	5	6
1:A:79:TYR:CG	1:A:108:VAL:HG21	0.44	2.48	14	5
1:A:53:SER:HB2	1:A:61:TRP:CZ2	0.44	2.48	5	1
1:A:79:TYR:CD1	1:A:108:VAL:HG21	0.44	2.48	16	1
1:A:35:ARG:HG2	1:A:36:LEU:O	0.44	2.12	14	2
1:A:81:VAL:O	1:A:88:LYS:HE2	0.43	2.14	18	4
1:A:65:LYS:H	1:A:87:ASN:ND2	0.43	2.12	6	1
1:A:27:ALA:HA	1:A:31:LYS:O	0.43	2.14	13	1
1:A:26:ASP:O	1:A:29:ASP:HB3	0.42	2.14	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:GLU:O	1:A:135:LEU:HG	0.42	2.15	13	2
1:A:105:ASN:O	1:A:109:GLU:HG3	0.42	2.14	8	1
1:A:109:GLU:HB3	1:A:113:ARG:NH2	0.42	2.30	1	1
1:A:87:ASN:N	1:A:87:ASN:HD22	0.42	2.13	15	1
1:A:98:GLU:H	1:A:98:GLU:CD	0.41	2.22	13	1
1:A:52:LEU:O	1:A:56:ILE:HG22	0.41	2.16	4	1
1:A:23:THR:HB	1:A:61:TRP:O	0.40	2.15	17	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	112/146 (77%)	110±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	100	100
All	All	2240/2920 (77%)	2201 (98%)	39 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	105/138 (76%)	103±1 (98±1%)	2±1 (2±1%)	45	90
All	All	2100/2760 (76%)	2053 (98%)	47 (2%)	45	90

All 19 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	45	LYS	16

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Mol	Chain	Res	Type	Models (Total)
1	A	98	GLU	4
1	A	39	ASN	3
1	A	131	GLU	3
1	A	62	SER	3
1	A	130	THR	2
1	A	72	LYS	2
1	A	58	LEU	2
1	A	31	LYS	2
1	A	51	LYS	1
1	A	100	SER	1
1	A	25	LYS	1
1	A	134	GLU	1
1	A	46	LYS	1
1	A	33	LYS	1
1	A	97	ARG	1
1	A	88	LYS	1
1	A	87	ASN	1
1	A	113	ARG	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

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 95% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	2014
Number of shifts mapped to atoms	1972
Number of unparsed shifts	0
Number of shifts with mapping errors	42
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 42 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	ASP	H	8.688	0.02	1
1	A	146	LYS	H	8.402	0.02	1
1	A	146	ILE	H	8.07	0.02	1
1	A	146	GLU	H	8.002	0.02	1
1	A	146	GLY	H	8.457	0.02	1
1	A	146	ILE	HA	3.902	0.02	1
1	A	146	ASP	HA	4.712	0.02	1
1	A	146	LYS	HA	4.249	0.02	1
1	A	146	PHE	HA	4.551	0.02	1
1	A	146	GLU	HA	4.488	0.02	1
1	A	146	GLY	HA2	3.881	0.02	2
1	A	146	GLY	HA3	3.881	0.02	2
1	A	146	ILE	HB	1.973	0.02	1
1	A	146	ASP	HB2	2.632	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	LYS	HB2	1.743	0.02	2
1	A	146	PHE	HB2	3.114	0.02	2
1	A	146	GLU	HB2	1.99	0.02	2
1	A	146	ASP	HB3	2.75	0.02	2
1	A	146	PHE	HB3	3.028	0.02	2
1	A	146	GLU	HB3	1.99	0.02	2
1	A	146	ILE	C	175.1	0.3	1
1	A	146	ASP	C	175.62	0.3	1
1	A	146	LYS	C	176.49	0.3	1
1	A	146	PHE	C	175.3	0.3	1
1	A	146	GLU	C	176.35	0.3	1
1	A	146	GLY	C	174.49	0.3	1
1	A	146	ILE	CA	60.49	0.3	1
1	A	146	ASP	CA	54.45	0.3	1
1	A	146	LYS	CA	56.87	0.3	1
1	A	146	PHE	CA	58.03	0.3	1
1	A	146	GLU	CA	56.43	0.3	1
1	A	146	GLY	CA	45.52	0.3	1
1	A	146	ILE	CB	38.91	0.3	1
1	A	146	ASP	CB	41.57	0.3	1
1	A	146	LYS	CB	32.93	0.3	1
1	A	146	PHE	CB	38.95	0.3	1
1	A	146	GLU	CB	30.49	0.3	1
1	A	146	ASP	N	125.858	0.2	1
1	A	146	LYS	N	122.382	0.2	1
1	A	146	ILE	N	120.472	0.2	1
1	A	146	GLU	N	121.72	0.2	1
1	A	146	GLY	N	111.37	0.2	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	152	-0.09 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	146	0.27 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	150	0.04 ± 0.10	None needed (< 0.5 ppm)
^{15}N	144	0.84 ± 0.23	Should be applied

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 95%, i.e. 1554 atoms were assigned a chemical shift out of a possible 1635. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	557/558 (100%)	225/225 (100%)	223/224 (100%)	109/109 (100%)
Sidechain	883/950 (93%)	602/619 (97%)	271/301 (90%)	10/30 (33%)
Aromatic	114/127 (90%)	57/61 (93%)	55/62 (89%)	2/4 (50%)
Overall	1554/1635 (95%)	884/905 (98%)	549/587 (94%)	121/143 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1972 atoms were assigned a chemical shift out of a possible 2125. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	719/727 (99%)	290/293 (99%)	290/292 (99%)	139/142 (98%)
Sidechain	1112/1194 (93%)	758/779 (97%)	343/380 (90%)	11/35 (31%)
Aromatic	141/204 (69%)	71/99 (72%)	68/89 (76%)	2/16 (12%)
Overall	1972/2125 (93%)	1119/1171 (96%)	701/761 (92%)	152/193 (79%)

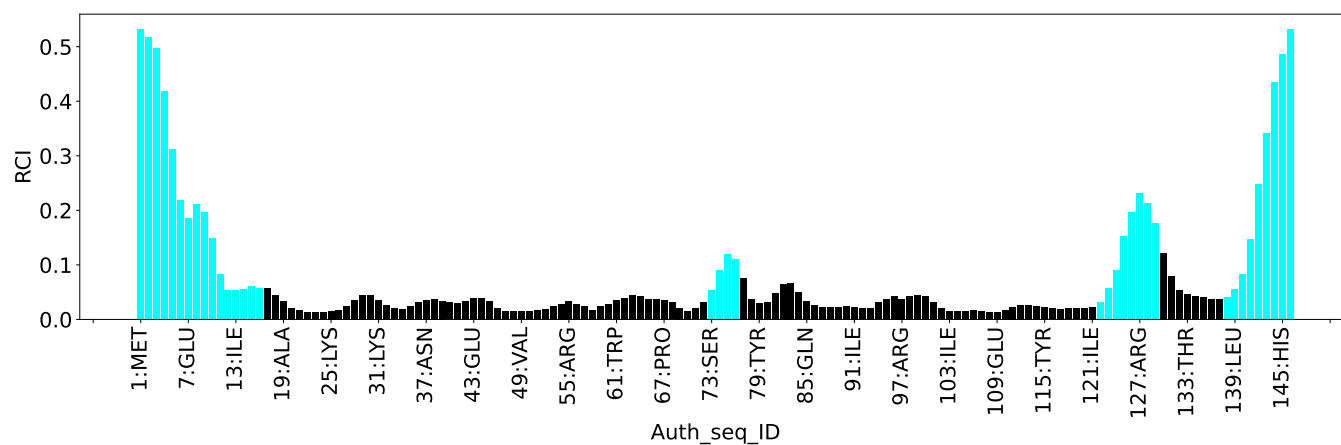
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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	4797
Intra-residue ($ i-j =0$)	1502
Sequential ($ i-j =1$)	974
Medium range ($ i-j >1$ and $ i-j <5$)	843
Long range ($ i-j \geq 5$)	1392
Inter-chain	0
Hydrogen bond restraints	86
Disulfide bond restraints	0
Total dihedral-angle restraints	297
Number of unmapped restraints	0
Number of restraints per residue	34.9
Number of long range restraints per residue ¹	9.8

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)	82.5	0.2
0.2-0.5 (Medium)	172.4	0.5
>0.5 (Large)	146.2	2.27

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	4.3	3.57
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

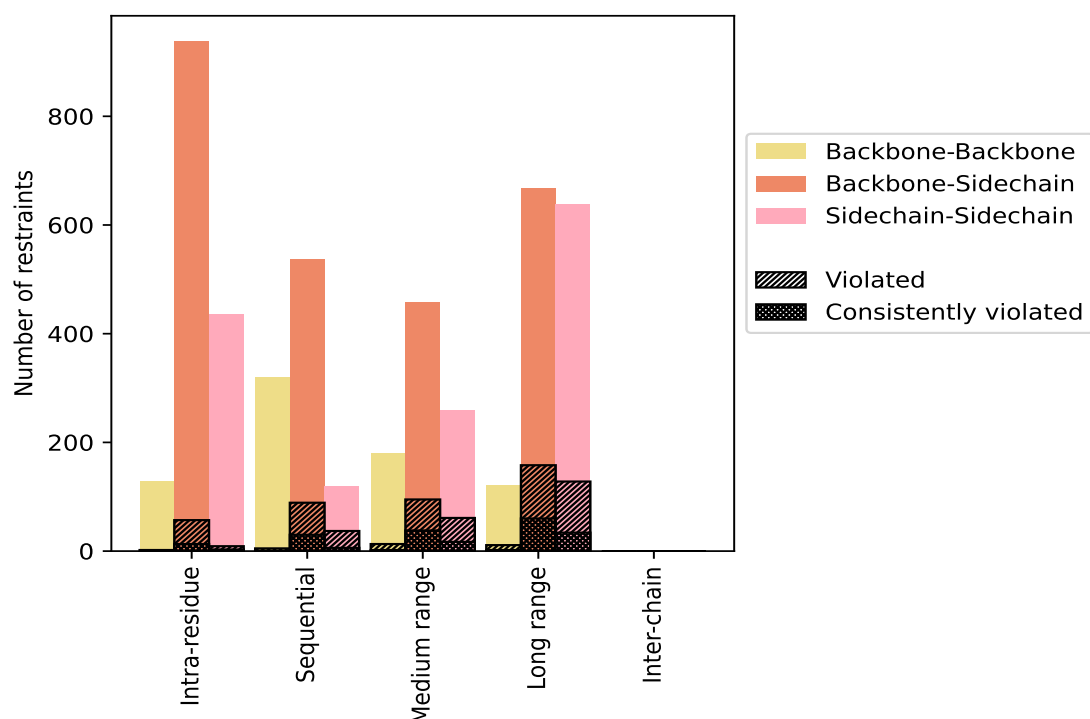
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1502	31.3	68	4.5	1.4	16	1.1	0.3
Backbone-Backbone	128	2.7	2	1.6	0.0	0	0.0	0.0
Backbone-Sidechain	938	19.6	57	6.1	1.2	13	1.4	0.3
Sidechain-Sidechain	436	9.1	9	2.1	0.2	3	0.7	0.1
Sequential ($i-j =1$)	974	20.3	131	13.4	2.7	37	3.8	0.8
Backbone-Backbone	319	6.6	5	1.6	0.1	1	0.3	0.0
Backbone-Sidechain	536	11.2	89	16.6	1.9	30	5.6	0.6
Sidechain-Sidechain	119	2.5	37	31.1	0.8	6	5.0	0.1
Medium range ($i-j >1$ & $i-j <5$)	843	17.6	169	20.0	3.5	57	6.8	1.2
Backbone-Backbone	179	3.7	13	7.3	0.3	2	1.1	0.0
Backbone-Sidechain	405	8.4	95	23.5	2.0	38	9.4	0.8
Sidechain-Sidechain	259	5.4	61	23.6	1.3	17	6.6	0.4
Long range ($i-j \geq 5$)	1392	29.0	297	21.3	6.2	96	6.9	2.0
Backbone-Backbone	120	2.5	11	9.2	0.2	2	1.7	0.0
Backbone-Sidechain	634	13.2	158	24.9	3.3	60	9.5	1.3
Sidechain-Sidechain	638	13.3	128	20.1	2.7	34	5.3	0.7
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	86	1.8	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	4797	100.0	665	13.9	13.9	206	4.3	4.3
Backbone-Backbone	746	15.6	31	4.2	0.6	5	0.7	0.1
Backbone-Sidechain	2599	54.2	399	15.4	8.3	141	5.4	2.9
Sidechain-Sidechain	1452	30.3	235	16.2	4.9	60	4.1	1.3

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	43	67	104	180	0	394	0.48	1.88	0.32	0.39
2	45	66	112	195	0	418	0.47	1.92	0.32	0.38
3	43	69	109	183	0	404	0.48	2.04	0.32	0.4
4	44	62	126	183	0	415	0.46	1.72	0.31	0.39
5	43	67	107	182	0	399	0.48	2.05	0.32	0.4
6	42	63	109	198	0	412	0.48	1.82	0.32	0.39
7	41	69	108	187	0	405	0.48	2.12	0.33	0.39
8	45	68	114	188	0	415	0.47	1.92	0.32	0.36
9	43	70	115	181	0	409	0.46	1.92	0.32	0.34
10	45	68	108	175	0	396	0.47	2.17	0.32	0.4

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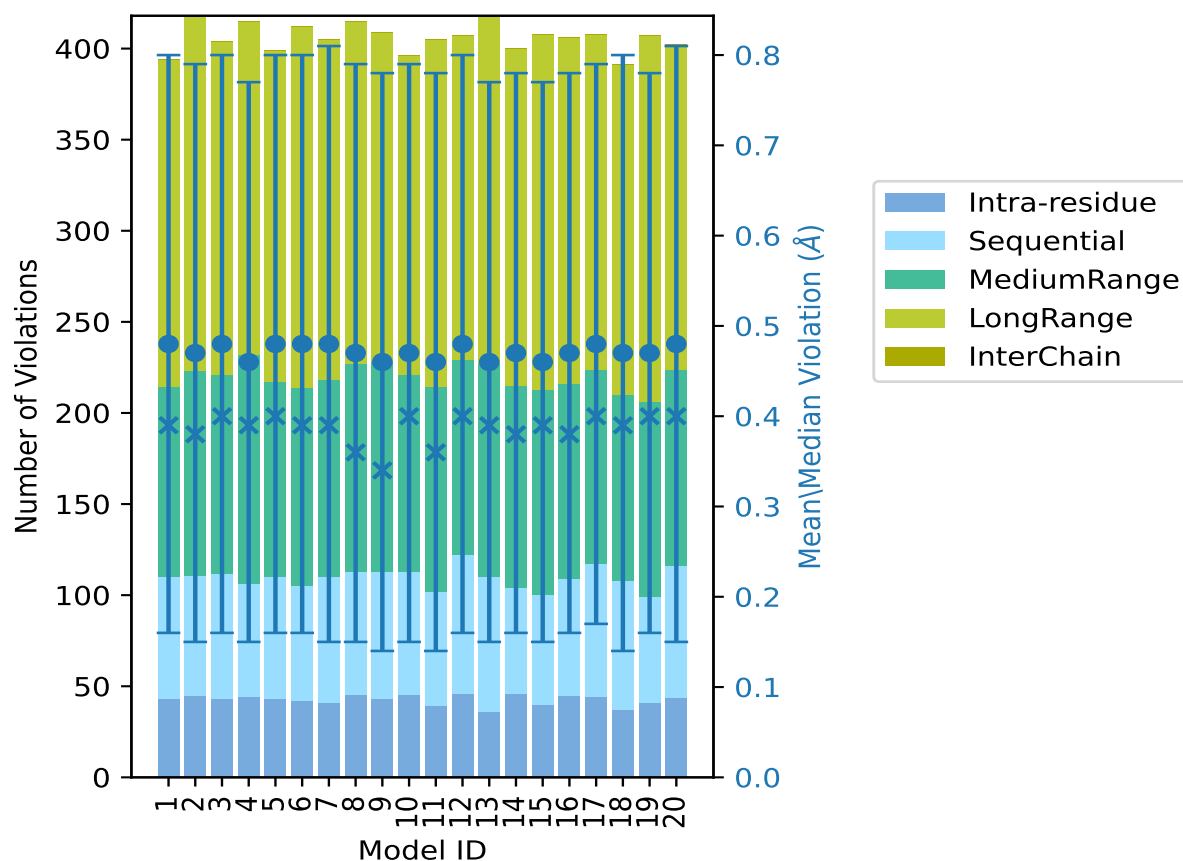
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	39	63	112	191	0	405	0.46	1.86	0.32	0.36
12	46	76	107	178	0	407	0.48	2.01	0.32	0.4
13	36	74	117	191	0	418	0.46	1.92	0.31	0.39
14	46	58	111	185	0	400	0.47	1.69	0.31	0.38
15	40	60	113	195	0	408	0.46	1.57	0.31	0.39
16	45	64	107	190	0	406	0.47	2.27	0.31	0.38
17	44	73	107	184	0	408	0.48	2.21	0.31	0.4
18	37	71	102	181	0	391	0.47	2.05	0.33	0.39
19	41	58	107	201	0	407	0.47	1.83	0.31	0.4
20	44	72	108	178	0	402	0.48	2.05	0.33	0.4

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

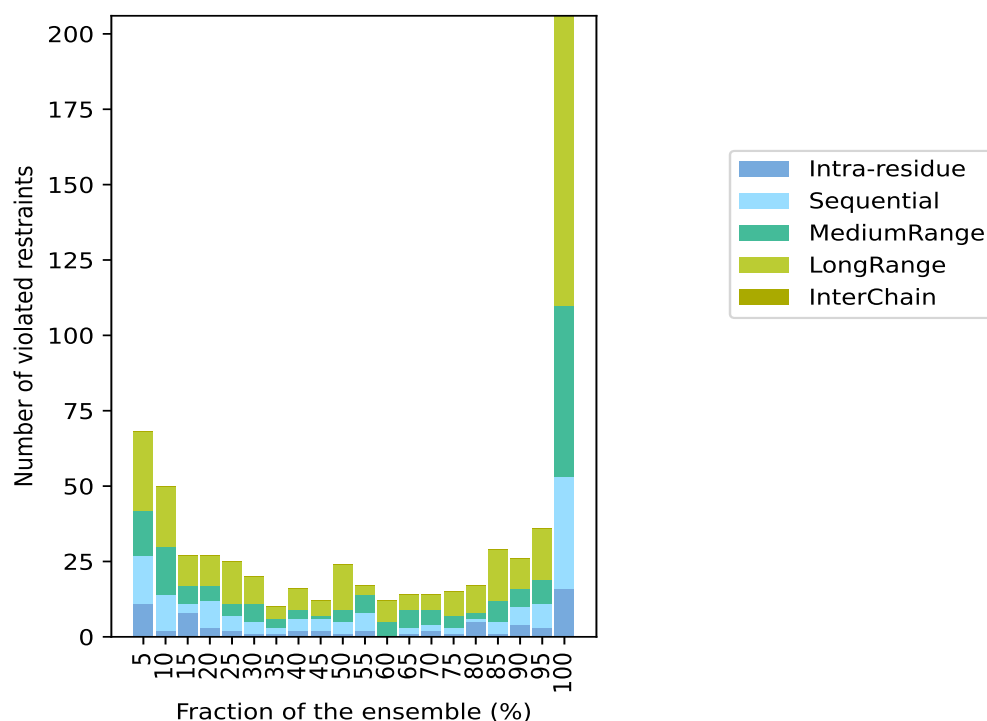
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 4046(IR:1434, SQ:843, MR:674, LR:1095, IC:0) restraints are 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	%
11	16	15	26	0	68	1	5.0
2	12	16	20	0	50	2	10.0
8	3	6	10	0	27	3	15.0
3	9	5	10	0	27	4	20.0
2	5	4	14	0	25	5	25.0
1	4	6	9	0	20	6	30.0
1	2	3	4	0	10	7	35.0
2	4	3	7	0	16	8	40.0
2	4	1	5	0	12	9	45.0
1	4	4	15	0	24	10	50.0
2	6	6	3	0	17	11	55.0
0	0	5	7	0	12	12	60.0
1	2	6	5	0	14	13	65.0
2	2	5	5	0	14	14	70.0
1	2	4	8	0	15	15	75.0
5	1	2	9	0	17	16	80.0
1	4	7	17	0	29	17	85.0
4	6	6	10	0	26	18	90.0
3	8	8	17	0	36	19	95.0
16	37	57	96	0	206	20	100.0

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

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

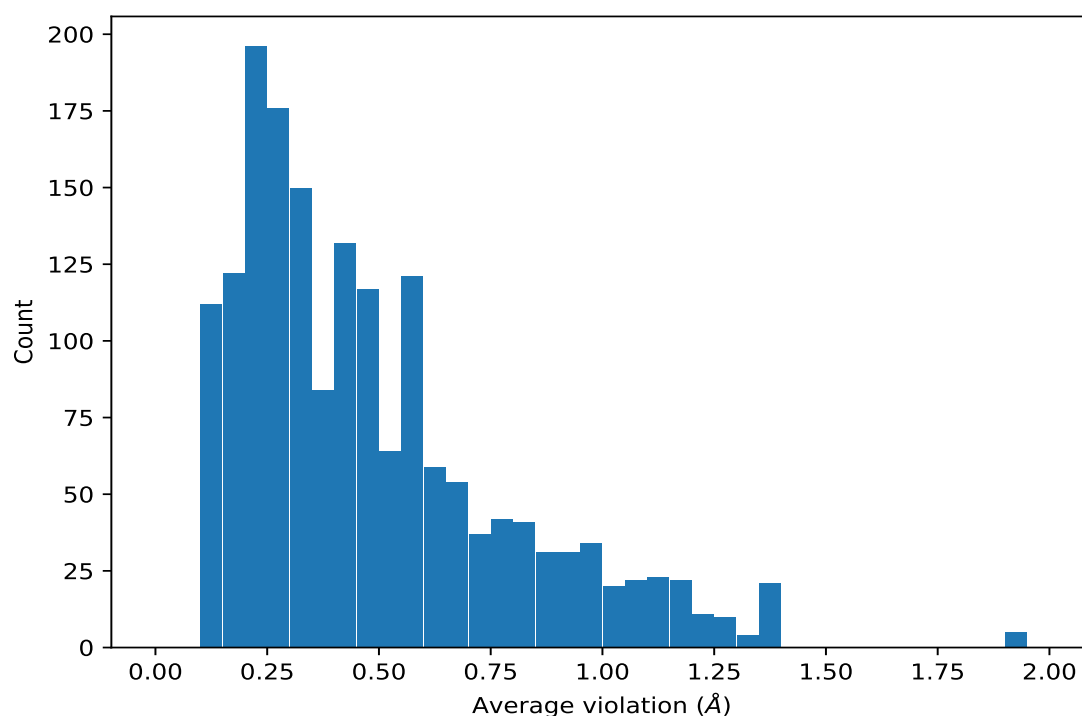
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG23	20	1.95	0.17	1.92
(2,3993)	1:83:A:GLY:HA2	1:66:A:ILE:HG23	20	1.95	0.17	1.92
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG22	20	1.95	0.17	1.92
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG21	20	1.95	0.17	1.92
(2,3993)	1:83:A:GLY:HA2	1:66:A:ILE:HG21	20	1.95	0.17	1.92
(2,3855)	1:121:A:ILE:HD11	1:108:A:VAL:HG21	20	1.38	0.09	1.37
(2,3855)	1:121:A:ILE:HD12	1:108:A:VAL:HG22	20	1.38	0.09	1.37
(2,3855)	1:81:A:VAL:HG21	1:108:A:VAL:HG21	20	1.38	0.09	1.37
(2,3855)	1:81:A:VAL:HG21	1:108:A:VAL:HG23	20	1.38	0.09	1.37
(2,3855)	1:121:A:ILE:HD11	1:108:A:VAL:HG23	20	1.38	0.09	1.37
(2,3855)	1:121:A:ILE:HD13	1:108:A:VAL:HG21	20	1.38	0.09	1.37
(2,3855)	1:121:A:ILE:HD12	1:108:A:VAL:HG23	20	1.38	0.09	1.37
(2,3855)	1:121:A:ILE:HD13	1:108:A:VAL:HG22	20	1.38	0.09	1.37
(2,3855)	1:121:A:ILE:HD13	1:108:A:VAL:HG23	20	1.38	0.09	1.37
(2,3855)	1:81:A:VAL:HG23	1:108:A:VAL:HG23	20	1.38	0.09	1.37
(2,3855)	1:81:A:VAL:HG22	1:108:A:VAL:HG22	20	1.38	0.09	1.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3855)	1:81:A:VAL:HG23	1:108:A:VAL:HG21	20	1.38	0.09	1.37
(2,1071)	1:119:A:ILE:HG23	1:117:A:SER:H	20	1.36	0.13	1.39
(2,1071)	1:119:A:ILE:HG22	1:117:A:SER:H	20	1.36	0.13	1.39
(2,1071)	1:119:A:ILE:HG21	1:117:A:SER:H	20	1.36	0.13	1.39
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG23	20	1.36	0.12	1.33
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG21	20	1.36	0.12	1.33
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG22	20	1.36	0.12	1.33
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG22	20	1.36	0.12	1.33
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG23	20	1.36	0.12	1.33
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG21	20	1.36	0.12	1.33
(2,1410)	1:119:A:ILE:HG21	1:116:A:THR:H	20	1.33	0.14	1.36
(2,1410)	1:119:A:ILE:HG23	1:116:A:THR:H	20	1.33	0.14	1.36
(2,1410)	1:119:A:ILE:HG22	1:116:A:THR:H	20	1.33	0.14	1.36
(2,1410)	1:52:A:LEU:HD21	1:116:A:THR:H	20	1.33	0.14	1.36
(2,889)	1:91:A:ILE:HD13	1:87:A:ASN:H	20	1.28	0.12	1.28
(2,889)	1:91:A:ILE:HD12	1:87:A:ASN:H	20	1.28	0.12	1.28
(2,889)	1:63:A:LEU:HD23	1:87:A:ASN:H	20	1.28	0.12	1.28
(2,889)	1:91:A:ILE:HD11	1:87:A:ASN:H	20	1.28	0.12	1.28
(2,889)	1:63:A:LEU:HD22	1:87:A:ASN:H	20	1.28	0.12	1.28
(2,1075)	1:119:A:ILE:HG21	1:115:A:TYR:H	20	1.27	0.19	1.32
(2,1075)	1:119:A:ILE:HG23	1:115:A:TYR:H	20	1.27	0.19	1.32
(2,1075)	1:52:A:LEU:HD11	1:115:A:TYR:H	20	1.27	0.19	1.32
(2,1075)	1:119:A:ILE:HG22	1:115:A:TYR:H	20	1.27	0.19	1.32
(2,1075)	1:52:A:LEU:HD21	1:115:A:TYR:H	20	1.27	0.19	1.32
(2,2197)	1:24:A:ILE:HG23	1:62:A:SER:HA	20	1.23	0.08	1.21
(2,2197)	1:24:A:ILE:HG22	1:62:A:SER:HA	20	1.23	0.08	1.21
(2,2197)	1:24:A:ILE:HG21	1:62:A:SER:HA	20	1.23	0.08	1.21
(2,1412)	1:119:A:ILE:HG21	1:114:A:GLU:H	20	1.22	0.16	1.28
(2,1412)	1:94:A:LEU:HD13	1:114:A:GLU:H	20	1.22	0.16	1.28
(2,1412)	1:94:A:LEU:HD12	1:114:A:GLU:H	20	1.22	0.16	1.28
(2,1412)	1:119:A:ILE:HG23	1:114:A:GLU:H	20	1.22	0.16	1.28
(2,1412)	1:119:A:ILE:HG22	1:114:A:GLU:H	20	1.22	0.16	1.28
(2,1412)	1:108:A:VAL:HG12	1:114:A:GLU:H	20	1.22	0.16	1.28
(2,1412)	1:108:A:VAL:HG13	1:114:A:GLU:H	20	1.22	0.16	1.28
(2,1412)	1:94:A:LEU:HD11	1:114:A:GLU:H	20	1.22	0.16	1.28
(2,1638)	1:24:A:ILE:HG23	1:62:A:SER:H	20	1.2	0.09	1.19
(2,1638)	1:24:A:ILE:HG21	1:62:A:SER:H	20	1.2	0.09	1.19
(2,1638)	1:24:A:ILE:HG22	1:62:A:SER:H	20	1.2	0.09	1.19
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD13	20	1.2	0.14	1.21
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD11	20	1.2	0.14	1.21
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD12	20	1.2	0.14	1.21
(2,4084)	1:56:A:ILE:H	1:93:A:ILE:HD13	20	1.2	0.14	1.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD11	20	1.19	0.1	1.21
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD12	20	1.19	0.1	1.21
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD13	20	1.19	0.1	1.21
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD12	20	1.18	0.16	1.19
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD13	20	1.18	0.16	1.19
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD11	20	1.18	0.16	1.19
(2,1652)	1:112:A:LEU:HD11	1:110:A:LYS:H	20	1.17	0.1	1.16
(2,1652)	1:112:A:LEU:HD13	1:110:A:LYS:H	20	1.17	0.1	1.16
(2,1652)	1:111:A:LEU:HD11	1:110:A:LYS:H	20	1.17	0.1	1.16
(2,1652)	1:112:A:LEU:HD12	1:110:A:LYS:H	20	1.17	0.1	1.16
(2,1652)	1:95:A:LEU:HD12	1:110:A:LYS:H	20	1.17	0.1	1.16
(2,1652)	1:111:A:LEU:HD13	1:110:A:LYS:H	20	1.17	0.1	1.16
(2,4384)	1:34:A:ILE:HG21	1:33:A:LYS:HB3	20	1.16	0.12	1.18
(2,4384)	1:34:A:ILE:HG23	1:33:A:LYS:HB3	20	1.16	0.12	1.18
(2,4384)	1:34:A:ILE:HG22	1:33:A:LYS:HB3	20	1.16	0.12	1.18
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD13	20	1.14	0.07	1.14
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD12	20	1.14	0.07	1.14
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD11	20	1.14	0.07	1.14
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB3	20	1.14	0.25	1.2
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB2	20	1.14	0.25	1.2
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB1	20	1.14	0.25	1.2
(2,4161)	1:89:A:LYS:HE2	1:93:A:ILE:HD11	20	1.13	0.27	1.18
(2,4161)	1:70:A:PHE:HB2	1:71:A:ILE:HD11	20	1.13	0.27	1.18
(2,4161)	1:70:A:PHE:HB2	1:71:A:ILE:HD12	20	1.13	0.27	1.18
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD13	20	1.13	0.27	1.18
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD12	20	1.13	0.27	1.18
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD11	20	1.13	0.27	1.18
(2,4161)	1:89:A:LYS:HE2	1:93:A:ILE:HD12	20	1.13	0.27	1.18
(2,4161)	1:70:A:PHE:HB2	1:71:A:ILE:HD13	20	1.13	0.27	1.18
(2,4161)	1:89:A:LYS:HE2	1:93:A:ILE:HD13	20	1.13	0.27	1.18
(2,1392)	1:119:A:ILE:HD12	1:116:A:THR:H	20	1.09	0.08	1.1
(2,1392)	1:119:A:ILE:HD11	1:116:A:THR:H	20	1.09	0.08	1.1
(2,1392)	1:119:A:ILE:HD13	1:116:A:THR:H	20	1.09	0.08	1.1
(2,3243)	1:63:A:LEU:HB2	1:61:A:TRP:HB2	20	1.07	0.06	1.08
(2,3243)	1:56:A:ILE:HD13	1:61:A:TRP:HB2	20	1.07	0.06	1.08
(2,3243)	1:56:A:ILE:HD11	1:61:A:TRP:HB2	20	1.07	0.06	1.08
(2,3243)	1:56:A:ILE:HD12	1:61:A:TRP:HB2	20	1.07	0.06	1.08
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD13	20	1.06	0.14	1.1
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD12	20	1.06	0.14	1.1
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD11	20	1.06	0.14	1.1
(2,2377)	1:52:A:LEU:HD13	1:115:A:TYR:HA	20	1.06	0.21	1.08
(2,2377)	1:52:A:LEU:HD11	1:115:A:TYR:HA	20	1.06	0.21	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2377)	1:52:A:LEU:HD23	1:115:A:TYR:HA	20	1.06	0.21	1.08
(2,2377)	1:52:A:LEU:HD12	1:115:A:TYR:HA	20	1.06	0.21	1.08
(2,2377)	1:52:A:LEU:HD21	1:115:A:TYR:HA	20	1.06	0.21	1.08
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD23	20	1.05	0.16	1.06
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD23	20	1.05	0.16	1.06
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD21	20	1.05	0.16	1.06
(2,3788)	1:53:A:SER:HA	1:94:A:LEU:HD23	20	1.05	0.16	1.06
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD22	20	1.05	0.16	1.06
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD21	20	1.05	0.16	1.06
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD22	20	1.05	0.16	1.06
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD12	20	1.04	0.06	1.03
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD11	20	1.04	0.06	1.03
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD13	20	1.04	0.06	1.03
(2,4122)	1:22:A:VAL:HA	1:66:A:ILE:HD11	20	1.01	0.11	0.98
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD11	20	1.01	0.11	0.98
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD12	20	1.01	0.11	0.98
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD13	20	1.01	0.11	0.98
(2,4122)	1:22:A:VAL:HA	1:66:A:ILE:HD12	20	1.01	0.11	0.98
(2,1643)	1:91:A:ILE:HG22	1:93:A:ILE:H	20	1.01	0.06	1.03
(2,1643)	1:91:A:ILE:HG23	1:93:A:ILE:H	20	1.01	0.06	1.03
(2,1643)	1:91:A:ILE:HG21	1:93:A:ILE:H	20	1.01	0.06	1.03
(2,1643)	1:94:A:LEU:HD23	1:93:A:ILE:H	20	1.01	0.06	1.03
(2,1643)	1:94:A:LEU:HD21	1:93:A:ILE:H	20	1.01	0.06	1.03
(2,344)	1:108:A:VAL:HG11	1:71:A:ILE:H	20	1.01	0.17	1.04
(2,344)	1:108:A:VAL:HG13	1:71:A:ILE:H	20	1.01	0.17	1.04
(2,344)	1:108:A:VAL:HG12	1:71:A:ILE:H	20	1.01	0.17	1.04
(2,344)	1:119:A:ILE:HG23	1:71:A:ILE:H	20	1.01	0.17	1.04
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG23	20	1.01	0.08	0.98
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG21	20	1.01	0.08	0.98
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG22	20	1.01	0.08	0.98
(2,867)	1:64:A:VAL:HG12	1:88:A:LYS:H	20	0.99	0.1	0.99
(2,867)	1:64:A:VAL:HG13	1:88:A:LYS:H	20	0.99	0.1	0.99
(2,867)	1:99:A:ILE:HG22	1:88:A:LYS:H	20	0.99	0.1	0.99
(2,867)	1:64:A:VAL:HG11	1:88:A:LYS:H	20	0.99	0.1	0.99
(2,867)	1:99:A:ILE:HG21	1:88:A:LYS:H	20	0.99	0.1	0.99
(2,867)	1:99:A:ILE:HG23	1:88:A:LYS:H	20	0.99	0.1	0.99
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD13	20	0.98	0.11	0.96
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD13	20	0.98	0.11	0.96
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD11	20	0.98	0.11	0.96
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD12	20	0.98	0.11	0.96
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD11	20	0.98	0.11	0.96
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD12	20	0.98	0.11	0.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2373)	1:36:A:LEU:HD23	1:21:A:TYR:HA	20	0.98	0.09	1.01
(2,2373)	1:36:A:LEU:HD21	1:21:A:TYR:HA	20	0.98	0.09	1.01
(2,2373)	1:36:A:LEU:HD22	1:21:A:TYR:HA	20	0.98	0.09	1.01
(2,2373)	1:66:A:ILE:HD13	1:21:A:TYR:HA	20	0.98	0.09	1.01
(2,2373)	1:66:A:ILE:HD12	1:21:A:TYR:HA	20	0.98	0.09	1.01
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	20	0.98	0.16	1.0
(2,761)	1:107:A:ASP:HB3	1:103:A:ILE:H	20	0.98	0.16	1.0
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD12	20	0.96	0.12	0.98
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD11	20	0.96	0.12	0.98
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD13	20	0.96	0.12	0.98
(2,3333)	1:115:A:TYR:H	1:52:A:LEU:HD21	20	0.96	0.12	0.98
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD12	20	0.96	0.16	0.99
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD11	20	0.96	0.16	0.99
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD13	20	0.96	0.16	0.99
(2,4190)	1:64:A:VAL:HG23	1:24:A:ILE:HG21	20	0.96	0.14	0.96
(2,4190)	1:64:A:VAL:HG21	1:24:A:ILE:HG23	20	0.96	0.14	0.96
(2,4190)	1:64:A:VAL:HG21	1:24:A:ILE:HG21	20	0.96	0.14	0.96
(2,4190)	1:64:A:VAL:HG22	1:24:A:ILE:HG23	20	0.96	0.14	0.96
(2,4190)	1:64:A:VAL:HG23	1:24:A:ILE:HG23	20	0.96	0.14	0.96
(2,4190)	1:64:A:VAL:HG23	1:24:A:ILE:HG22	20	0.96	0.14	0.96
(2,4190)	1:64:A:VAL:HG22	1:24:A:ILE:HG21	20	0.96	0.14	0.96
(2,4190)	1:64:A:VAL:HG21	1:24:A:ILE:HG22	20	0.96	0.14	0.96
(2,2873)	1:91:A:ILE:HD13	1:87:A:ASN:HB2	20	0.95	0.11	0.96
(2,2873)	1:91:A:ILE:HD12	1:87:A:ASN:HB2	20	0.95	0.11	0.96
(2,2873)	1:91:A:ILE:HD11	1:87:A:ASN:HB2	20	0.95	0.11	0.96
(2,1059)	1:91:A:ILE:HG22	1:91:A:ILE:H	20	0.95	0.02	0.96
(2,1059)	1:91:A:ILE:HG23	1:91:A:ILE:H	20	0.95	0.02	0.96
(2,1059)	1:91:A:ILE:HG21	1:91:A:ILE:H	20	0.95	0.02	0.96
(2,168)	1:119:A:ILE:HG23	1:122:A:ILE:H	20	0.93	0.11	0.94
(2,168)	1:119:A:ILE:HG22	1:122:A:ILE:H	20	0.93	0.11	0.94
(2,168)	1:119:A:ILE:HG21	1:122:A:ILE:H	20	0.93	0.11	0.94
(2,4209)	1:68:A:PHE:HA	1:91:A:ILE:HD13	20	0.92	0.12	0.92
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD12	20	0.92	0.12	0.92
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD13	20	0.92	0.12	0.92
(2,4209)	1:68:A:PHE:HA	1:91:A:ILE:HD12	20	0.92	0.12	0.92
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD11	20	0.92	0.12	0.92
(2,4209)	1:68:A:PHE:HA	1:91:A:ILE:HD11	20	0.92	0.12	0.92
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD23	20	0.91	0.08	0.92
(2,3689)	1:94:A:LEU:H	1:111:A:LEU:HD23	20	0.91	0.08	0.92
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD22	20	0.91	0.08	0.92
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD21	20	0.91	0.08	0.92
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	20	0.91	0.17	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1402)	1:99:A:ILE:HG22	1:101:A:ASN:HD22	20	0.91	0.18	0.9
(2,1402)	1:99:A:ILE:HG21	1:101:A:ASN:HD22	20	0.91	0.18	0.9
(2,1402)	1:99:A:ILE:HG23	1:101:A:ASN:HD22	20	0.91	0.18	0.9
(2,1404)	1:122:A:ILE:HD12	1:37:A:ASN:HD22	20	0.88	0.37	0.92
(2,1404)	1:35:A:ARG:HG2	1:37:A:ASN:HD22	20	0.88	0.37	0.92
(2,1404)	1:69:A:ILE:HD12	1:37:A:ASN:HD22	20	0.88	0.37	0.92
(2,1404)	1:122:A:ILE:HD13	1:37:A:ASN:HD22	20	0.88	0.37	0.92
(2,1404)	1:122:A:ILE:HD11	1:37:A:ASN:HD22	20	0.88	0.37	0.92
(2,1404)	1:69:A:ILE:HD11	1:37:A:ASN:HD22	20	0.88	0.37	0.92
(2,1404)	1:69:A:ILE:HD13	1:37:A:ASN:HD22	20	0.88	0.37	0.92
(2,2156)	1:121:A:ILE:HD11	1:121:A:ILE:HA	20	0.87	0.03	0.88
(2,2156)	1:121:A:ILE:HD12	1:121:A:ILE:HA	20	0.87	0.03	0.88
(2,2156)	1:122:A:ILE:HD11	1:121:A:ILE:HA	20	0.87	0.03	0.88
(2,2156)	1:122:A:ILE:HD13	1:121:A:ILE:HA	20	0.87	0.03	0.88
(2,2156)	1:121:A:ILE:HD13	1:121:A:ILE:HA	20	0.87	0.03	0.88
(2,4244)	1:81:A:VAL:HG11	1:80:A:PHE:HA	20	0.87	0.03	0.87
(2,4244)	1:81:A:VAL:HG13	1:80:A:PHE:HA	20	0.87	0.03	0.87
(2,4244)	1:81:A:VAL:HG12	1:80:A:PHE:HA	20	0.87	0.03	0.87
(2,600)	1:91:A:ILE:HD13	1:69:A:ILE:H	20	0.86	0.13	0.88
(2,600)	1:91:A:ILE:HD12	1:69:A:ILE:H	20	0.86	0.13	0.88
(2,600)	1:91:A:ILE:HD11	1:69:A:ILE:H	20	0.86	0.13	0.88
(2,3857)	1:66:A:ILE:HG23	1:49:A:VAL:HG21	20	0.86	0.08	0.87
(2,3857)	1:66:A:ILE:HG21	1:49:A:VAL:HG22	20	0.86	0.08	0.87
(2,3857)	1:24:A:ILE:HG22	1:49:A:VAL:HG22	20	0.86	0.08	0.87
(2,3857)	1:24:A:ILE:HG21	1:49:A:VAL:HG23	20	0.86	0.08	0.87
(2,3857)	1:66:A:ILE:HG23	1:49:A:VAL:HG23	20	0.86	0.08	0.87
(2,3857)	1:66:A:ILE:HG22	1:49:A:VAL:HG23	20	0.86	0.08	0.87
(2,3857)	1:66:A:ILE:HG21	1:49:A:VAL:HG21	20	0.86	0.08	0.87
(2,3857)	1:66:A:ILE:HG22	1:49:A:VAL:HG22	20	0.86	0.08	0.87
(2,3857)	1:24:A:ILE:HG22	1:49:A:VAL:HG21	20	0.86	0.08	0.87
(2,3857)	1:66:A:ILE:HG22	1:49:A:VAL:HG21	20	0.86	0.08	0.87
(2,3857)	1:24:A:ILE:HG21	1:49:A:VAL:HG22	20	0.86	0.08	0.87
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG21	20	0.84	0.09	0.83
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG23	20	0.84	0.09	0.83
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG22	20	0.84	0.09	0.83
(2,4178)	1:28:A:LEU:HB3	1:24:A:ILE:HG22	20	0.84	0.09	0.83
(2,1257)	1:108:A:VAL:HG13	1:113:A:ARG:H	20	0.84	0.12	0.84
(2,1257)	1:108:A:VAL:HG12	1:113:A:ARG:H	20	0.84	0.12	0.84
(2,1257)	1:108:A:VAL:HG11	1:113:A:ARG:H	20	0.84	0.12	0.84
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	20	0.82	0.09	0.8
(2,4394)	1:71:A:ILE:HG22	1:80:A:PHE:HB3	20	0.82	0.06	0.82
(2,4394)	1:71:A:ILE:HG21	1:80:A:PHE:HB3	20	0.82	0.06	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4394)	1:71:A:ILE:HG23	1:80:A:PHE:HB3	20	0.82	0.06	0.82
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD12	20	0.81	0.07	0.8
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD11	20	0.81	0.07	0.8
(2,4131)	1:60:A:LEU:HA	1:24:A:ILE:HD12	20	0.81	0.07	0.8
(2,4131)	1:60:A:LEU:HA	1:24:A:ILE:HD13	20	0.81	0.07	0.8
(2,4131)	1:60:A:LEU:HA	1:24:A:ILE:HD11	20	0.81	0.07	0.8
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD13	20	0.81	0.07	0.8
(2,1497)	1:81:A:VAL:HG12	1:83:A:GLY:H	20	0.8	0.13	0.76
(2,1497)	1:81:A:VAL:HG11	1:83:A:GLY:H	20	0.8	0.13	0.76
(2,1497)	1:81:A:VAL:HG13	1:83:A:GLY:H	20	0.8	0.13	0.76
(2,1051)	1:106:A:VAL:HG23	1:109:A:GLU:H	20	0.8	0.1	0.8
(2,1051)	1:106:A:VAL:HG21	1:109:A:GLU:H	20	0.8	0.1	0.8
(2,1051)	1:106:A:VAL:HG22	1:109:A:GLU:H	20	0.8	0.1	0.8
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG23	20	0.8	0.3	0.88
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG22	20	0.8	0.3	0.88
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG21	20	0.8	0.3	0.88
(2,3905)	1:80:A:PHE:HE1	1:102:A:VAL:HG21	20	0.8	0.3	0.88
(2,3905)	1:80:A:PHE:HE1	1:102:A:VAL:HG22	20	0.8	0.3	0.88
(2,3905)	1:80:A:PHE:HE1	1:102:A:VAL:HG23	20	0.8	0.3	0.88
(2,1666)	1:121:A:ILE:HD12	1:121:A:ILE:H	20	0.78	0.07	0.8
(2,1666)	1:121:A:ILE:HD13	1:121:A:ILE:H	20	0.78	0.07	0.8
(2,1666)	1:121:A:ILE:HD11	1:121:A:ILE:H	20	0.78	0.07	0.8
(2,1666)	1:122:A:ILE:HD12	1:121:A:ILE:H	20	0.78	0.07	0.8
(2,1666)	1:122:A:ILE:HD13	1:121:A:ILE:H	20	0.78	0.07	0.8
(2,4105)	1:59:A:TYR:HE1	1:93:A:ILE:HD12	20	0.78	0.2	0.8
(2,4105)	1:79:A:TYR:HD1	1:71:A:ILE:HD11	20	0.78	0.2	0.8
(2,4105)	1:59:A:TYR:HE2	1:93:A:ILE:HD11	20	0.78	0.2	0.8
(2,4105)	1:79:A:TYR:HD1	1:71:A:ILE:HD12	20	0.78	0.2	0.8
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD11	20	0.78	0.2	0.8
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD12	20	0.78	0.2	0.8
(2,4105)	1:79:A:TYR:HD1	1:71:A:ILE:HD13	20	0.78	0.2	0.8
(2,4105)	1:59:A:TYR:HE1	1:93:A:ILE:HD13	20	0.78	0.2	0.8
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD13	20	0.78	0.2	0.8
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD12	20	0.76	0.12	0.8
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD11	20	0.76	0.12	0.8
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD11	20	0.76	0.12	0.8
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD13	20	0.76	0.12	0.8
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD12	20	0.76	0.12	0.8
(2,4518)	1:76:A:ILE:HD11	1:80:A:PHE:HZ	20	0.75	0.17	0.72
(2,4518)	1:76:A:ILE:HD12	1:80:A:PHE:HZ	20	0.75	0.17	0.72
(2,4518)	1:76:A:ILE:HD13	1:80:A:PHE:HZ	20	0.75	0.17	0.72
(2,4518)	1:102:A:VAL:HG22	1:80:A:PHE:HZ	20	0.75	0.17	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4518)	1:102:A:VAL:HG23	1:80:A:PHE:HZ	20	0.75	0.17	0.72
(2,4518)	1:102:A:VAL:HG21	1:80:A:PHE:HZ	20	0.75	0.17	0.72
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD21	20	0.74	0.12	0.74
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD22	20	0.74	0.12	0.74
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD23	20	0.74	0.12	0.74
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD21	20	0.74	0.12	0.74
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD22	20	0.74	0.12	0.74
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD23	20	0.74	0.12	0.74
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD13	20	0.74	0.1	0.73
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD12	20	0.74	0.1	0.73
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD11	20	0.74	0.1	0.73
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD12	20	0.74	0.17	0.75
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD13	20	0.74	0.17	0.75
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD11	20	0.74	0.17	0.75
(2,4351)	1:111:A:LEU:HD21	1:91:A:ILE:HD12	20	0.73	0.19	0.76
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD11	20	0.73	0.19	0.76
(2,4351)	1:111:A:LEU:HD21	1:91:A:ILE:HD11	20	0.73	0.19	0.76
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD12	20	0.73	0.19	0.76
(2,4351)	1:111:A:LEU:HD23	1:91:A:ILE:HD11	20	0.73	0.19	0.76
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD13	20	0.73	0.19	0.76
(2,4351)	1:111:A:LEU:HD23	1:91:A:ILE:HD12	20	0.73	0.19	0.76
(2,4351)	1:111:A:LEU:HD23	1:91:A:ILE:HD13	20	0.73	0.19	0.76
(2,1398)	1:111:A:LEU:HD23	1:114:A:GLU:H	20	0.73	0.14	0.76
(2,1398)	1:111:A:LEU:HD21	1:114:A:GLU:H	20	0.73	0.14	0.76
(2,1398)	1:119:A:ILE:HD11	1:114:A:GLU:H	20	0.73	0.14	0.76
(2,1398)	1:119:A:ILE:HD13	1:114:A:GLU:H	20	0.73	0.14	0.76
(2,1398)	1:119:A:ILE:HD12	1:114:A:GLU:H	20	0.73	0.14	0.76
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD13	20	0.71	0.12	0.76
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD12	20	0.71	0.12	0.76
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD11	20	0.71	0.12	0.76
(2,596)	1:28:A:LEU:HD12	1:50:A:GLU:H	20	0.7	0.06	0.72
(2,596)	1:28:A:LEU:HD11	1:50:A:GLU:H	20	0.7	0.06	0.72
(2,596)	1:28:A:LEU:HD13	1:50:A:GLU:H	20	0.7	0.06	0.72
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD13	20	0.7	0.09	0.7
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD11	20	0.7	0.09	0.7
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD12	20	0.7	0.09	0.7
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD23	20	0.7	0.16	0.72
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD21	20	0.7	0.16	0.72
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD22	20	0.7	0.16	0.72
(2,1896)	1:94:A:LEU:HD13	1:93:A:ILE:HA	20	0.68	0.09	0.69
(2,1896)	1:60:A:LEU:HD13	1:93:A:ILE:HA	20	0.68	0.09	0.69
(2,1896)	1:60:A:LEU:HD12	1:93:A:ILE:HA	20	0.68	0.09	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1896)	1:60:A:LEU:HD11	1:93:A:ILE:HA	20	0.68	0.09	0.69
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	20	0.68	0.07	0.68
(2,1550)	1:50:A:GLU:HG2	1:46:A:LYS:H	20	0.68	0.07	0.68
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	20	0.67	0.08	0.68
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	20	0.67	0.16	0.72
(2,665)	1:115:A:TYR:HE2	1:112:A:LEU:H	20	0.67	0.16	0.72
(2,665)	1:115:A:TYR:HE1	1:112:A:LEU:H	20	0.67	0.16	0.72
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD22	20	0.66	0.06	0.66
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD21	20	0.66	0.06	0.66
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD23	20	0.66	0.06	0.66
(2,235)	1:25:A:LYS:HB3	1:27:A:ALA:H	20	0.66	0.14	0.62
(2,235)	1:31:A:LYS:HB3	1:27:A:ALA:H	20	0.66	0.14	0.62
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	20	0.65	0.18	0.66
(2,1486)	1:69:A:ILE:HG13	1:83:A:GLY:H	20	0.65	0.18	0.66
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	20	0.65	0.09	0.67
(2,237)	1:90:A:ALA:HB1	1:93:A:ILE:H	20	0.65	0.09	0.67
(2,237)	1:90:A:ALA:HB3	1:93:A:ILE:H	20	0.65	0.09	0.67
(2,2382)	1:103:A:ILE:HG13	1:107:A:ASP:HA	20	0.64	0.13	0.67
(2,2382)	1:28:A:LEU:HD21	1:47:A:ASP:HA	20	0.64	0.13	0.67
(2,2382)	1:103:A:ILE:HG23	1:107:A:ASP:HA	20	0.64	0.13	0.67
(2,2382)	1:103:A:ILE:HG21	1:107:A:ASP:HA	20	0.64	0.13	0.67
(2,2382)	1:103:A:ILE:HG22	1:107:A:ASP:HA	20	0.64	0.13	0.67
(2,2382)	1:28:A:LEU:HD23	1:47:A:ASP:HA	20	0.64	0.13	0.67
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD1	20	0.64	0.19	0.65
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD2	20	0.64	0.19	0.65
(2,4458)	1:20:A:GLU:HB2	1:21:A:TYR:HD1	20	0.64	0.19	0.65
(2,4458)	1:20:A:GLU:HB2	1:21:A:TYR:HD2	20	0.64	0.19	0.65
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG21	20	0.64	0.07	0.64
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	20	0.64	0.07	0.64
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG22	20	0.64	0.07	0.64
(2,1610)	1:95:A:LEU:HD23	1:110:A:LYS:H	20	0.64	0.14	0.63
(2,1610)	1:95:A:LEU:HD21	1:110:A:LYS:H	20	0.64	0.14	0.63
(2,1610)	1:95:A:LEU:HD22	1:110:A:LYS:H	20	0.64	0.14	0.63
(2,1501)	1:95:A:LEU:HD12	1:96:A:GLY:H	20	0.64	0.08	0.64
(2,1501)	1:95:A:LEU:HD11	1:96:A:GLY:H	20	0.64	0.08	0.64
(2,1501)	1:95:A:LEU:HD13	1:96:A:GLY:H	20	0.64	0.08	0.64
(2,248)	1:36:A:LEU:HD12	1:36:A:LEU:H	20	0.62	0.06	0.62
(2,248)	1:36:A:LEU:HD11	1:36:A:LEU:H	20	0.62	0.06	0.62
(2,248)	1:36:A:LEU:HD13	1:36:A:LEU:H	20	0.62	0.06	0.62
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD13	20	0.62	0.03	0.61
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD12	20	0.62	0.03	0.61
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD11	20	0.62	0.03	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG23	20	0.61	0.18	0.62
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG21	20	0.61	0.18	0.62
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG22	20	0.61	0.18	0.62
(2,4026)	1:52:A:LEU:HB3	1:66:A:ILE:HG23	20	0.61	0.18	0.62
(2,4107)	1:21:A:TYR:HD1	1:34:A:ILE:HD11	20	0.61	0.1	0.57
(2,4107)	1:21:A:TYR:HD2	1:34:A:ILE:HD11	20	0.61	0.1	0.57
(2,4107)	1:41:A:TYR:HD1	1:34:A:ILE:HD13	20	0.61	0.1	0.57
(2,4107)	1:21:A:TYR:HD2	1:34:A:ILE:HD13	20	0.61	0.1	0.57
(2,4107)	1:41:A:TYR:HD2	1:34:A:ILE:HD12	20	0.61	0.1	0.57
(2,4107)	1:41:A:TYR:HD2	1:34:A:ILE:HD11	20	0.61	0.1	0.57
(2,4107)	1:21:A:TYR:HD2	1:34:A:ILE:HD12	20	0.61	0.1	0.57
(2,4107)	1:41:A:TYR:HD2	1:34:A:ILE:HD13	20	0.61	0.1	0.57
(2,4107)	1:41:A:TYR:HD1	1:34:A:ILE:HD12	20	0.61	0.1	0.57
(2,4107)	1:41:A:TYR:HD1	1:34:A:ILE:HD11	20	0.61	0.1	0.57
(2,4107)	1:21:A:TYR:HD1	1:34:A:ILE:HD12	20	0.61	0.1	0.57
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD23	20	0.61	0.11	0.61
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD21	20	0.61	0.11	0.61
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD22	20	0.61	0.11	0.61
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG12	20	0.6	0.26	0.66
(2,3708)	1:64:A:VAL:H	1:64:A:VAL:HG11	20	0.6	0.26	0.66
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG13	20	0.6	0.26	0.66
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG11	20	0.6	0.26	0.66
(2,3708)	1:64:A:VAL:H	1:64:A:VAL:HG13	20	0.6	0.26	0.66
(2,3708)	1:64:A:VAL:H	1:64:A:VAL:HG12	20	0.6	0.26	0.66
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB1	20	0.6	0.08	0.62
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB3	20	0.6	0.08	0.62
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB2	20	0.6	0.08	0.62
(2,1066)	1:99:A:ILE:HD13	1:97:A:ARG:H	20	0.6	0.2	0.6
(2,1066)	1:99:A:ILE:HD12	1:97:A:ARG:H	20	0.6	0.2	0.6
(2,1066)	1:99:A:ILE:HD11	1:97:A:ARG:H	20	0.6	0.2	0.6
(2,550)	1:24:A:ILE:HG13	1:63:A:LEU:H	20	0.6	0.03	0.6
(2,550)	1:60:A:LEU:HB2	1:63:A:LEU:H	20	0.6	0.03	0.6
(2,550)	1:25:A:LYS:HG3	1:63:A:LEU:H	20	0.6	0.03	0.6
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	20	0.6	0.09	0.62
(2,2863)	1:22:A:VAL:HG12	1:26:A:ASP:HB3	20	0.6	0.09	0.62
(2,2863)	1:22:A:VAL:HG13	1:26:A:ASP:HB3	20	0.6	0.09	0.62
(2,2194)	1:28:A:LEU:HD12	1:54:A:SER:HA	20	0.58	0.18	0.54
(2,2194)	1:28:A:LEU:HD11	1:54:A:SER:HA	20	0.58	0.18	0.54
(2,2194)	1:58:A:LEU:HD21	1:54:A:SER:HA	20	0.58	0.18	0.54
(2,2194)	1:28:A:LEU:HD13	1:54:A:SER:HA	20	0.58	0.18	0.54
(2,2194)	1:58:A:LEU:HD22	1:54:A:SER:HA	20	0.58	0.18	0.54
(2,2194)	1:58:A:LEU:HD23	1:54:A:SER:HA	20	0.58	0.18	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1226)	1:95:A:LEU:HD12	1:95:A:LEU:H	20	0.58	0.06	0.6
(2,1226)	1:95:A:LEU:HD11	1:95:A:LEU:H	20	0.58	0.06	0.6
(2,1226)	1:95:A:LEU:HD13	1:95:A:LEU:H	20	0.58	0.06	0.6
(2,1226)	1:91:A:ILE:HG23	1:95:A:LEU:H	20	0.58	0.06	0.6
(2,1226)	1:91:A:ILE:HG22	1:95:A:LEU:H	20	0.58	0.06	0.6
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD13	20	0.58	0.05	0.6
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD12	20	0.58	0.05	0.6
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD11	20	0.58	0.05	0.6
(2,4006)	1:80:A:PHE:HB3	1:99:A:ILE:HG21	20	0.58	0.25	0.55
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG23	20	0.58	0.25	0.55
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG22	20	0.58	0.25	0.55
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG21	20	0.58	0.25	0.55
(2,4006)	1:80:A:PHE:HB3	1:99:A:ILE:HG23	20	0.58	0.25	0.55
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG23	20	0.57	0.17	0.6
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG22	20	0.57	0.17	0.6
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG21	20	0.57	0.17	0.6
(2,3966)	1:98:A:GLU:HA	1:99:A:ILE:HG22	20	0.57	0.17	0.6
(2,3966)	1:98:A:GLU:HA	1:99:A:ILE:HG21	20	0.57	0.17	0.6
(2,3966)	1:98:A:GLU:HA	1:99:A:ILE:HG23	20	0.57	0.17	0.6
(2,607)	1:66:A:ILE:HG21	1:64:A:VAL:H	20	0.57	0.14	0.54
(2,607)	1:66:A:ILE:HG22	1:64:A:VAL:H	20	0.57	0.14	0.54
(2,607)	1:66:A:ILE:HG23	1:64:A:VAL:H	20	0.57	0.14	0.54
(2,1557)	1:24:A:ILE:HD13	1:61:A:TRP:HE1	20	0.57	0.15	0.6
(2,1557)	1:24:A:ILE:HD12	1:61:A:TRP:HE1	20	0.57	0.15	0.6
(2,1557)	1:24:A:ILE:HD11	1:61:A:TRP:HE1	20	0.57	0.15	0.6
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	20	0.57	0.12	0.57
(2,116)	1:17:A:SER:HB3	1:120:A:PHE:H	20	0.57	0.12	0.57
(2,116)	1:82:A:SER:HB3	1:120:A:PHE:H	20	0.57	0.12	0.57
(2,331)	1:33:A:LYS:HB3	1:32:A:LEU:H	20	0.56	0.14	0.59
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	20	0.56	0.14	0.59
(2,331)	1:31:A:LYS:HD3	1:32:A:LEU:H	20	0.56	0.14	0.59
(2,610)	1:24:A:ILE:HG21	1:63:A:LEU:H	20	0.56	0.09	0.56
(2,610)	1:24:A:ILE:HG23	1:63:A:LEU:H	20	0.56	0.09	0.56
(2,610)	1:24:A:ILE:HG22	1:63:A:LEU:H	20	0.56	0.09	0.56
(2,77)	1:56:A:ILE:HD13	1:61:A:TRP:HE1	20	0.56	0.07	0.58
(2,77)	1:56:A:ILE:HD12	1:61:A:TRP:HE1	20	0.56	0.07	0.58
(2,77)	1:56:A:ILE:HD11	1:61:A:TRP:HE1	20	0.56	0.07	0.58
(2,245)	1:44:A:ILE:HD13	1:44:A:ILE:H	20	0.56	0.13	0.58
(2,245)	1:44:A:ILE:HD12	1:44:A:ILE:H	20	0.56	0.13	0.58
(2,245)	1:44:A:ILE:HD11	1:44:A:ILE:H	20	0.56	0.13	0.58
(2,245)	1:44:A:ILE:HG23	1:44:A:ILE:H	20	0.56	0.13	0.58
(2,245)	1:32:A:LEU:HD21	1:44:A:ILE:H	20	0.56	0.13	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,245)	1:32:A:LEU:HD22	1:44:A:ILE:H	20	0.56	0.13	0.58
(2,245)	1:32:A:LEU:HD23	1:44:A:ILE:H	20	0.56	0.13	0.58
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG11	20	0.55	0.07	0.54
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG12	20	0.55	0.07	0.54
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG13	20	0.55	0.07	0.54
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	20	0.55	0.09	0.58
(2,1818)	1:80:A:PHE:HB2	1:81:A:VAL:HA	20	0.55	0.09	0.58
(2,3501)	1:112:A:LEU:HA	1:121:A:ILE:HG13	20	0.54	0.14	0.52
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	20	0.54	0.14	0.52
(2,333)	1:56:A:ILE:HG21	1:61:A:TRP:H	20	0.54	0.04	0.54
(2,333)	1:56:A:ILE:HG22	1:61:A:TRP:H	20	0.54	0.04	0.54
(2,333)	1:56:A:ILE:HG23	1:61:A:TRP:H	20	0.54	0.04	0.54
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	20	0.53	0.19	0.56
(2,4254)	1:45:A:LYS:HG3	1:47:A:ASP:HB3	20	0.53	0.19	0.56
(2,4254)	1:46:A:LYS:HG2	1:47:A:ASP:HB3	20	0.53	0.19	0.56
(2,1256)	1:24:A:ILE:HG21	1:54:A:SER:H	20	0.53	0.14	0.54
(2,1256)	1:28:A:LEU:HD11	1:54:A:SER:H	20	0.53	0.14	0.54
(2,1256)	1:24:A:ILE:HG23	1:54:A:SER:H	20	0.53	0.14	0.54
(2,1256)	1:28:A:LEU:HD13	1:54:A:SER:H	20	0.53	0.14	0.54
(2,1256)	1:24:A:ILE:HG22	1:54:A:SER:H	20	0.53	0.14	0.54
(2,1256)	1:28:A:LEU:HD12	1:54:A:SER:H	20	0.53	0.14	0.54
(2,2163)	1:102:A:VAL:HG22	1:103:A:ILE:HA	20	0.53	0.2	0.52
(2,2163)	1:102:A:VAL:HG23	1:103:A:ILE:HA	20	0.53	0.2	0.52
(2,2163)	1:102:A:VAL:HG21	1:103:A:ILE:HA	20	0.53	0.2	0.52
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD23	20	0.53	0.18	0.6
(2,3685)	1:27:A:ALA:H	1:49:A:VAL:HG23	20	0.53	0.18	0.6
(2,3685)	1:27:A:ALA:H	1:49:A:VAL:HG21	20	0.53	0.18	0.6
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD21	20	0.53	0.18	0.6
(2,3685)	1:27:A:ALA:H	1:49:A:VAL:HG22	20	0.53	0.18	0.6
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD22	20	0.53	0.18	0.6
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	20	0.52	0.05	0.52
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	20	0.52	0.08	0.52
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	20	0.51	0.23	0.46
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE2	20	0.51	0.23	0.46
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	20	0.51	0.09	0.5
(2,3463)	1:87:A:ASN:HA	1:88:A:LYS:HG3	20	0.51	0.09	0.5
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG21	20	0.5	0.1	0.51
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG23	20	0.5	0.1	0.51
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG22	20	0.5	0.1	0.51
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	20	0.5	0.16	0.52
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG22	20	0.5	0.13	0.52
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG21	20	0.5	0.13	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG23	20	0.5	0.13	0.52
(2,3973)	1:81:A:VAL:HA	1:119:A:ILE:HG22	20	0.5	0.13	0.52
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	20	0.5	0.17	0.53
(2,4457)	1:20:A:GLU:HG3	1:21:A:TYR:HD2	20	0.5	0.17	0.53
(2,4457)	1:20:A:GLU:HG3	1:21:A:TYR:HD1	20	0.5	0.17	0.53
(2,4457)	1:43:A:GLU:HG3	1:41:A:TYR:HD2	20	0.5	0.17	0.53
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD2	20	0.5	0.17	0.53
(2,4457)	1:43:A:GLU:HG3	1:41:A:TYR:HD1	20	0.5	0.17	0.53
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD13	20	0.5	0.2	0.49
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD11	20	0.5	0.2	0.49
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD12	20	0.5	0.2	0.49
(2,1234)	1:94:A:LEU:HD23	1:56:A:ILE:H	20	0.49	0.09	0.51
(2,1234)	1:94:A:LEU:HD22	1:56:A:ILE:H	20	0.49	0.09	0.51
(2,1234)	1:94:A:LEU:HD21	1:56:A:ILE:H	20	0.49	0.09	0.51
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	20	0.48	0.05	0.46
(2,1240)	1:112:A:LEU:HD11	1:113:A:ARG:H	20	0.48	0.1	0.45
(2,1240)	1:112:A:LEU:HD13	1:113:A:ARG:H	20	0.48	0.1	0.45
(2,1240)	1:112:A:LEU:HD12	1:113:A:ARG:H	20	0.48	0.1	0.45
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG22	20	0.48	0.11	0.44
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG23	20	0.48	0.11	0.44
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG21	20	0.48	0.11	0.44
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD13	20	0.47	0.14	0.5
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD12	20	0.47	0.14	0.5
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD11	20	0.47	0.14	0.5
(2,4072)	1:94:A:LEU:H	1:93:A:ILE:HD13	20	0.47	0.14	0.5
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD11	20	0.47	0.05	0.49
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD13	20	0.47	0.05	0.49
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD12	20	0.47	0.05	0.49
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	20	0.47	0.08	0.47
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD13	20	0.46	0.08	0.46
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD12	20	0.46	0.08	0.46
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD11	20	0.46	0.08	0.46
(2,4125)	1:104:A:LEU:HA	1:103:A:ILE:HD13	20	0.46	0.08	0.46
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB3	20	0.46	0.21	0.42
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB2	20	0.46	0.21	0.42
(2,4222)	1:71:A:ILE:HB	1:73:A:SER:HB2	20	0.46	0.21	0.42
(2,4222)	1:75:A:GLU:HB3	1:73:A:SER:HB3	20	0.46	0.21	0.42
(2,1228)	1:123:A:LEU:HD21	1:124:A:SER:H	20	0.46	0.15	0.45
(2,1228)	1:122:A:ILE:HG22	1:124:A:SER:H	20	0.46	0.15	0.45
(2,1228)	1:123:A:LEU:HD22	1:124:A:SER:H	20	0.46	0.15	0.45
(2,1228)	1:123:A:LEU:HD23	1:124:A:SER:H	20	0.46	0.15	0.45
(2,1228)	1:122:A:ILE:HG21	1:124:A:SER:H	20	0.46	0.15	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1228)	1:122:A:ILE:HG23	1:124:A:SER:H	20	0.46	0.15	0.45
(2,4570)	1:60:A:LEU:HD21	1:86:A:TRP:HD1	20	0.46	0.11	0.46
(2,4570)	1:60:A:LEU:HD22	1:86:A:TRP:HD1	20	0.46	0.11	0.46
(2,4570)	1:60:A:LEU:HD23	1:86:A:TRP:HD1	20	0.46	0.11	0.46
(2,2364)	1:93:A:ILE:HG21	1:90:A:ALA:HA	20	0.45	0.12	0.44
(2,2364)	1:93:A:ILE:HG23	1:90:A:ALA:HA	20	0.45	0.12	0.44
(2,2364)	1:93:A:ILE:HG22	1:90:A:ALA:HA	20	0.45	0.12	0.44
(2,868)	1:23:A:THR:HG22	1:24:A:ILE:H	20	0.44	0.02	0.44
(2,868)	1:23:A:THR:HG21	1:24:A:ILE:H	20	0.44	0.02	0.44
(2,868)	1:23:A:THR:HG23	1:24:A:ILE:H	20	0.44	0.02	0.44
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	20	0.44	0.18	0.45
(2,1225)	1:95:A:LEU:HD21	1:95:A:LEU:H	20	0.44	0.1	0.43
(2,1225)	1:95:A:LEU:HD22	1:95:A:LEU:H	20	0.44	0.1	0.43
(2,1225)	1:95:A:LEU:HD23	1:95:A:LEU:H	20	0.44	0.1	0.43
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	20	0.44	0.17	0.46
(2,1632)	1:138:A:MET:HB3	1:136:A:SER:H	20	0.44	0.17	0.46
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	20	0.44	0.12	0.43
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG23	20	0.44	0.12	0.46
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG21	20	0.44	0.12	0.46
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG22	20	0.44	0.12	0.46
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	20	0.44	0.14	0.46
(2,1219)	1:45:A:LYS:HG3	1:47:A:ASP:H	20	0.44	0.14	0.46
(2,1219)	1:65:A:LYS:HD2	1:22:A:VAL:H	20	0.44	0.14	0.46
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD12	20	0.44	0.07	0.44
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD13	20	0.44	0.07	0.44
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD11	20	0.44	0.07	0.44
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD12	20	0.44	0.11	0.45
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD11	20	0.44	0.11	0.45
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD13	20	0.44	0.11	0.45
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD23	20	0.44	0.12	0.41
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD22	20	0.44	0.12	0.41
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD21	20	0.44	0.12	0.41
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	20	0.43	0.09	0.45
(2,1808)	1:92:A:SER:HB3	1:91:A:ILE:HA	20	0.43	0.09	0.45
(2,598)	1:24:A:ILE:HG22	1:52:A:LEU:H	20	0.43	0.11	0.44
(2,598)	1:24:A:ILE:HG21	1:52:A:LEU:H	20	0.43	0.11	0.44
(2,598)	1:24:A:ILE:HG23	1:52:A:LEU:H	20	0.43	0.11	0.44
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	20	0.43	0.08	0.44
(2,1686)	1:24:A:ILE:HG23	1:23:A:THR:HB	20	0.43	0.06	0.43
(2,1686)	1:24:A:ILE:HG22	1:23:A:THR:HB	20	0.43	0.06	0.43
(2,1686)	1:66:A:ILE:HG21	1:23:A:THR:HB	20	0.43	0.06	0.43
(2,1686)	1:24:A:ILE:HG21	1:23:A:THR:HB	20	0.43	0.06	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2081)	1:43:A:GLU:HG3	1:41:A:TYR:HA	20	0.43	0.09	0.44
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	20	0.43	0.09	0.44
(2,851)	1:106:A:VAL:HG13	1:108:A:VAL:H	20	0.42	0.06	0.42
(2,851)	1:106:A:VAL:HG11	1:108:A:VAL:H	20	0.42	0.06	0.42
(2,851)	1:106:A:VAL:HG12	1:108:A:VAL:H	20	0.42	0.06	0.42
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG22	20	0.42	0.09	0.42
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG21	20	0.42	0.09	0.42
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG23	20	0.42	0.09	0.42
(2,564)	1:104:A:LEU:HD22	1:79:A:TYR:H	20	0.41	0.12	0.43
(2,564)	1:104:A:LEU:HD23	1:79:A:TYR:H	20	0.41	0.12	0.43
(2,564)	1:104:A:LEU:HD13	1:79:A:TYR:H	20	0.41	0.12	0.43
(2,564)	1:104:A:LEU:HD21	1:79:A:TYR:H	20	0.41	0.12	0.43
(2,564)	1:104:A:LEU:HD12	1:79:A:TYR:H	20	0.41	0.12	0.43
(2,2874)	1:118:A:LEU:HD22	1:48:A:GLU:HG3	20	0.41	0.16	0.39
(2,2874)	1:118:A:LEU:HD21	1:48:A:GLU:HG3	20	0.41	0.16	0.39
(2,2874)	1:118:A:LEU:HD23	1:48:A:GLU:HG3	20	0.41	0.16	0.39
(2,2874)	1:49:A:VAL:HG23	1:48:A:GLU:HG3	20	0.41	0.16	0.39
(2,4519)	1:119:A:ILE:HG22	1:68:A:PHE:HD1	20	0.41	0.1	0.4
(2,4519)	1:119:A:ILE:HG21	1:68:A:PHE:HD2	20	0.41	0.1	0.4
(2,4519)	1:119:A:ILE:HG23	1:68:A:PHE:HD2	20	0.41	0.1	0.4
(2,4519)	1:119:A:ILE:HG23	1:68:A:PHE:HD1	20	0.41	0.1	0.4
(2,4519)	1:119:A:ILE:HG22	1:68:A:PHE:HD2	20	0.41	0.1	0.4
(2,4519)	1:119:A:ILE:HG21	1:68:A:PHE:HD1	20	0.41	0.1	0.4
(2,4519)	1:52:A:LEU:HD23	1:68:A:PHE:HD1	20	0.41	0.1	0.4
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD22	20	0.41	0.12	0.42
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD23	20	0.41	0.12	0.42
(2,3670)	1:103:A:ILE:H	1:104:A:LEU:HD23	20	0.41	0.12	0.42
(2,3670)	1:103:A:ILE:H	1:104:A:LEU:HD22	20	0.41	0.12	0.42
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD21	20	0.41	0.12	0.42
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	20	0.4	0.04	0.4
(2,3038)	1:90:A:ALA:H	1:89:A:LYS:HD2	20	0.4	0.04	0.4
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD13	20	0.4	0.12	0.38
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD12	20	0.4	0.12	0.38
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD13	20	0.4	0.12	0.38
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD11	20	0.4	0.12	0.38
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD11	20	0.4	0.12	0.38
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	20	0.4	0.06	0.43
(2,4046)	1:24:A:ILE:HD12	1:66:A:ILE:HG21	20	0.4	0.07	0.4
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG22	20	0.4	0.07	0.4
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG23	20	0.4	0.07	0.4
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG21	20	0.4	0.07	0.4
(2,4046)	1:24:A:ILE:HD13	1:66:A:ILE:HG22	20	0.4	0.07	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4046)	1:24:A:ILE:HD13	1:66:A:ILE:HG21	20	0.4	0.07	0.4
(2,4046)	1:24:A:ILE:HD12	1:66:A:ILE:HG22	20	0.4	0.07	0.4
(2,4046)	1:24:A:ILE:HD13	1:66:A:ILE:HG23	20	0.4	0.07	0.4
(2,4046)	1:24:A:ILE:HD12	1:66:A:ILE:HG23	20	0.4	0.07	0.4
(2,864)	1:111:A:LEU:HD11	1:111:A:LEU:H	20	0.4	0.03	0.4
(2,864)	1:111:A:LEU:HD13	1:111:A:LEU:H	20	0.4	0.03	0.4
(2,864)	1:111:A:LEU:HD12	1:111:A:LEU:H	20	0.4	0.03	0.4
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG23	20	0.39	0.13	0.4
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG22	20	0.39	0.13	0.4
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG21	20	0.39	0.13	0.4
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD11	20	0.38	0.06	0.38
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD13	20	0.38	0.06	0.38
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD12	20	0.38	0.06	0.38
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD22	20	0.37	0.1	0.38
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD21	20	0.37	0.1	0.38
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD23	20	0.37	0.1	0.38
(2,850)	1:139:A:LEU:HD11	1:140:A:GLU:H	20	0.36	0.11	0.36
(2,850)	1:139:A:LEU:HD12	1:140:A:GLU:H	20	0.36	0.11	0.36
(2,850)	1:22:A:VAL:HG22	1:26:A:ASP:H	20	0.36	0.11	0.36
(2,850)	1:139:A:LEU:HD23	1:140:A:GLU:H	20	0.36	0.11	0.36
(2,850)	1:139:A:LEU:HD13	1:140:A:GLU:H	20	0.36	0.11	0.36
(2,850)	1:22:A:VAL:HG21	1:26:A:ASP:H	20	0.36	0.11	0.36
(2,850)	1:139:A:LEU:HD21	1:140:A:GLU:H	20	0.36	0.11	0.36
(2,1056)	1:91:A:ILE:HG22	1:92:A:SER:H	20	0.36	0.07	0.36
(2,1056)	1:91:A:ILE:HG23	1:92:A:SER:H	20	0.36	0.07	0.36
(2,1056)	1:91:A:ILE:HG21	1:92:A:SER:H	20	0.36	0.07	0.36
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	20	0.36	0.05	0.34
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE2	20	0.36	0.05	0.34
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	20	0.35	0.06	0.37
(2,848)	1:27:A:ALA:HB1	1:26:A:ASP:H	20	0.34	0.12	0.36
(2,848)	1:27:A:ALA:HB3	1:26:A:ASP:H	20	0.34	0.12	0.36
(2,848)	1:27:A:ALA:HB2	1:26:A:ASP:H	20	0.34	0.12	0.36
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	20	0.34	0.12	0.36
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	20	0.34	0.12	0.36
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	20	0.34	0.12	0.36
(2,166)	1:22:A:VAL:HG11	1:31:A:LYS:H	20	0.34	0.12	0.36
(2,166)	1:22:A:VAL:HG12	1:31:A:LYS:H	20	0.34	0.12	0.36
(2,166)	1:22:A:VAL:HG13	1:31:A:LYS:H	20	0.34	0.12	0.36
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	20	0.34	0.07	0.36
(2,580)	1:46:A:LYS:HG3	1:51:A:LYS:H	20	0.34	0.07	0.36
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD11	20	0.34	0.04	0.34
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD13	20	0.34	0.04	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD12	20	0.34	0.04	0.34
(2,1541)	1:22:A:VAL:HB	1:30:A:GLY:H	20	0.34	0.1	0.36
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	20	0.34	0.1	0.36
(2,1180)	1:45:A:LYS:HE3	1:47:A:ASP:H	20	0.34	0.1	0.34
(2,1180)	1:26:A:ASP:HB3	1:22:A:VAL:H	20	0.34	0.1	0.34
(2,1180)	1:45:A:LYS:HE2	1:47:A:ASP:H	20	0.34	0.1	0.34
(2,874)	1:49:A:VAL:HG23	1:48:A:GLU:H	20	0.34	0.07	0.34
(2,874)	1:49:A:VAL:HG21	1:48:A:GLU:H	20	0.34	0.07	0.34
(2,874)	1:49:A:VAL:HG22	1:48:A:GLU:H	20	0.34	0.07	0.34
(2,1904)	1:56:A:ILE:HD13	1:53:A:SER:HA	20	0.33	0.07	0.34
(2,1904)	1:56:A:ILE:HD12	1:53:A:SER:HA	20	0.33	0.07	0.34
(2,1904)	1:56:A:ILE:HD11	1:53:A:SER:HA	20	0.33	0.07	0.34
(2,1236)	1:36:A:LEU:HD11	1:38:A:ASN:H	20	0.33	0.09	0.35
(2,1236)	1:19:A:ALA:HB1	1:38:A:ASN:H	20	0.33	0.09	0.35
(2,1236)	1:19:A:ALA:HB2	1:38:A:ASN:H	20	0.33	0.09	0.35
(2,1236)	1:36:A:LEU:HD13	1:38:A:ASN:H	20	0.33	0.09	0.35
(2,1236)	1:19:A:ALA:HB3	1:38:A:ASN:H	20	0.33	0.09	0.35
(2,1236)	1:36:A:LEU:HD12	1:38:A:ASN:H	20	0.33	0.09	0.35
(2,2376)	1:34:A:ILE:HD12	1:42:A:HIS:HA	20	0.33	0.05	0.32
(2,2376)	1:34:A:ILE:HD13	1:42:A:HIS:HA	20	0.33	0.05	0.32
(2,2376)	1:34:A:ILE:HD11	1:42:A:HIS:HA	20	0.33	0.05	0.32
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	20	0.33	0.08	0.32
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	20	0.32	0.08	0.32
(2,1027)	1:90:A:ALA:HB2	1:92:A:SER:H	20	0.32	0.09	0.28
(2,1027)	1:90:A:ALA:HB1	1:92:A:SER:H	20	0.32	0.09	0.28
(2,1027)	1:90:A:ALA:HB3	1:92:A:SER:H	20	0.32	0.09	0.28
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	20	0.31	0.05	0.32
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	20	0.31	0.02	0.3
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB3	20	0.31	0.09	0.32
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB2	20	0.31	0.09	0.32
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB1	20	0.31	0.09	0.32
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	20	0.3	0.07	0.31
(2,4236)	1:118:A:LEU:HD23	1:117:A:SER:HA	20	0.3	0.05	0.3
(2,4236)	1:118:A:LEU:HD22	1:117:A:SER:HA	20	0.3	0.05	0.3
(2,4236)	1:118:A:LEU:HD21	1:117:A:SER:HA	20	0.3	0.05	0.3
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	20	0.29	0.07	0.3
(2,145)	1:122:A:ILE:HG13	1:70:A:PHE:H	20	0.29	0.07	0.3
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	20	0.29	0.07	0.3
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	20	0.28	0.06	0.28
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG21	20	0.28	0.06	0.29
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG23	20	0.28	0.06	0.29
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG22	20	0.28	0.06	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE1	20	0.26	0.02	0.26
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE2	20	0.26	0.02	0.26
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD12	20	0.26	0.02	0.26
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD13	20	0.26	0.02	0.26
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD11	20	0.26	0.02	0.26
(2,1063)	1:23:A:THR:HG23	1:25:A:LYS:H	20	0.26	0.07	0.26
(2,1063)	1:23:A:THR:HG22	1:25:A:LYS:H	20	0.26	0.07	0.26
(2,1063)	1:23:A:THR:HG21	1:25:A:LYS:H	20	0.26	0.07	0.26
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD11	20	0.25	0.05	0.26
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD13	20	0.25	0.05	0.26
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD12	20	0.25	0.05	0.26
(2,4143)	1:81:A:VAL:HA	1:103:A:ILE:HD13	20	0.25	0.05	0.26
(2,1447)	1:22:A:VAL:HG21	1:23:A:THR:H	20	0.24	0.03	0.25
(2,1447)	1:22:A:VAL:HG23	1:23:A:THR:H	20	0.24	0.03	0.25
(2,1447)	1:22:A:VAL:HG22	1:23:A:THR:H	20	0.24	0.03	0.25
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE1	20	0.24	0.03	0.24
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE2	20	0.24	0.03	0.24
(2,1839)	1:76:A:ILE:HB	1:76:A:ILE:HA	20	0.24	0.01	0.24
(2,1839)	1:5:A:ILE:HB	1:5:A:ILE:HA	20	0.24	0.01	0.24
(2,2796)	1:76:A:ILE:HA	1:76:A:ILE:HB	20	0.24	0.01	0.24
(2,2796)	1:5:A:ILE:HA	1:5:A:ILE:HB	20	0.24	0.01	0.24
(2,34)	1:71:A:ILE:HG21	1:72:A:LYS:H	20	0.24	0.08	0.23
(2,34)	1:71:A:ILE:HG23	1:72:A:LYS:H	20	0.24	0.08	0.23
(2,34)	1:71:A:ILE:HG22	1:72:A:LYS:H	20	0.24	0.08	0.23
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	20	0.22	0.03	0.22
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	20	0.21	0.06	0.22
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	20	0.2	0.04	0.2
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG22	20	0.19	0.03	0.2
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG21	20	0.19	0.03	0.2
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG23	20	0.19	0.03	0.2
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	20	0.19	0.03	0.18
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	20	0.18	0.02	0.18
(2,3065)	1:70:A:PHE:HD1	1:81:A:VAL:HB	20	0.17	0.02	0.16
(2,3065)	1:70:A:PHE:HD2	1:81:A:VAL:HB	20	0.17	0.02	0.16
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE1	20	0.14	0.01	0.13
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE2	20	0.14	0.01	0.13
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	20	0.14	0.02	0.13
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	20	0.14	0.02	0.13
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD23	19	0.84	0.09	0.85
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD21	19	0.84	0.09	0.85
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD22	19	0.84	0.09	0.85
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG22	19	0.8	0.48	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG23	19	0.8	0.48	0.7
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG21	19	0.8	0.48	0.7
(2,4000)	1:72:A:LYS:HE2	1:121:A:ILE:HG22	19	0.8	0.48	0.7
(2,3838)	1:31:A:LYS:HG2	1:22:A:VAL:HG12	19	0.79	0.31	0.83
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG11	19	0.79	0.31	0.83
(2,3838)	1:31:A:LYS:HG2	1:22:A:VAL:HG13	19	0.79	0.31	0.83
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG13	19	0.79	0.31	0.83
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG12	19	0.79	0.31	0.83
(2,560)	1:95:A:LEU:HD11	1:104:A:LEU:H	19	0.65	0.32	0.77
(2,560)	1:95:A:LEU:HD13	1:104:A:LEU:H	19	0.65	0.32	0.77
(2,560)	1:95:A:LEU:HD12	1:104:A:LEU:H	19	0.65	0.32	0.77
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	19	0.57	0.1	0.59
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD23	19	0.56	0.22	0.61
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD21	19	0.56	0.22	0.61
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD22	19	0.56	0.22	0.61
(2,2174)	1:99:A:ILE:HD12	1:89:A:LYS:HA	19	0.55	0.18	0.6
(2,2174)	1:60:A:LEU:HG	1:59:A:TYR:HA	19	0.55	0.18	0.6
(2,2174)	1:99:A:ILE:HD11	1:89:A:LYS:HA	19	0.55	0.18	0.6
(2,2174)	1:99:A:ILE:HD13	1:89:A:LYS:HA	19	0.55	0.18	0.6
(2,3635)	1:52:A:LEU:HD12	1:56:A:ILE:HG12	19	0.48	0.18	0.47
(2,3635)	1:52:A:LEU:HD13	1:56:A:ILE:HG12	19	0.48	0.18	0.47
(2,3635)	1:52:A:LEU:HD11	1:56:A:ILE:HG12	19	0.48	0.18	0.47
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD21	19	0.47	0.18	0.46
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD22	19	0.47	0.18	0.46
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD23	19	0.47	0.18	0.46
(2,3703)	1:70:A:PHE:HD2	1:112:A:LEU:HD23	19	0.47	0.18	0.46
(2,3703)	1:70:A:PHE:HD2	1:112:A:LEU:HD22	19	0.47	0.18	0.46
(2,3703)	1:70:A:PHE:HD2	1:112:A:LEU:HD21	19	0.47	0.18	0.46
(2,1866)	1:139:A:LEU:HB2	1:136:A:SER:HB3	19	0.46	0.16	0.49
(2,1866)	1:139:A:LEU:HB2	1:136:A:SER:HB2	19	0.46	0.16	0.49
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	19	0.46	0.16	0.49
(2,83)	1:34:A:ILE:HD12	1:43:A:GLU:H	19	0.45	0.07	0.45
(2,83)	1:34:A:ILE:HD13	1:43:A:GLU:H	19	0.45	0.07	0.45
(2,83)	1:34:A:ILE:HD11	1:43:A:GLU:H	19	0.45	0.07	0.45
(2,3247)	1:60:A:LEU:HD21	1:89:A:LYS:HB3	19	0.45	0.14	0.47
(2,3247)	1:60:A:LEU:HD22	1:89:A:LYS:HB3	19	0.45	0.14	0.47
(2,3247)	1:60:A:LEU:HD23	1:89:A:LYS:HB3	19	0.45	0.14	0.47
(2,3344)	1:119:A:ILE:H	1:119:A:ILE:HG12	19	0.44	0.1	0.42
(2,3344)	1:70:A:PHE:HD2	1:119:A:ILE:HG12	19	0.44	0.1	0.42
(2,3344)	1:70:A:PHE:HD1	1:119:A:ILE:HG12	19	0.44	0.1	0.42
(2,3344)	1:14:A:PHE:HE2	1:71:A:ILE:HG13	19	0.44	0.1	0.42
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD11	19	0.44	0.12	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4120)	1:21:A:TYR:HA	1:34:A:ILE:HD11	19	0.44	0.12	0.43
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD12	19	0.44	0.12	0.43
(2,4120)	1:21:A:TYR:HA	1:34:A:ILE:HD13	19	0.44	0.12	0.43
(2,4120)	1:21:A:TYR:HA	1:34:A:ILE:HD12	19	0.44	0.12	0.43
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD13	19	0.44	0.12	0.43
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	19	0.43	0.17	0.47
(2,3072)	1:88:A:LYS:H	1:85:A:GLN:HG2	19	0.43	0.17	0.47
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD12	19	0.41	0.11	0.42
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD13	19	0.41	0.11	0.42
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD11	19	0.41	0.11	0.42
(2,583)	1:94:A:LEU:HD23	1:55:A:ARG:H	19	0.4	0.11	0.38
(2,583)	1:94:A:LEU:HD22	1:55:A:ARG:H	19	0.4	0.11	0.38
(2,583)	1:94:A:LEU:HD21	1:55:A:ARG:H	19	0.4	0.11	0.38
(2,396)	1:68:A:PHE:HZ	1:68:A:PHE:H	19	0.38	0.09	0.42
(2,396)	1:120:A:PHE:HE1	1:68:A:PHE:H	19	0.38	0.09	0.42
(2,396)	1:120:A:PHE:HE2	1:68:A:PHE:H	19	0.38	0.09	0.42
(2,396)	1:21:A:TYR:HE2	1:68:A:PHE:H	19	0.38	0.09	0.42
(2,1626)	1:135:A:LEU:HD22	1:136:A:SER:H	19	0.38	0.13	0.36
(2,1626)	1:139:A:LEU:HD11	1:136:A:SER:H	19	0.38	0.13	0.36
(2,1626)	1:135:A:LEU:HD11	1:136:A:SER:H	19	0.38	0.13	0.36
(2,1626)	1:139:A:LEU:HD13	1:136:A:SER:H	19	0.38	0.13	0.36
(2,1626)	1:135:A:LEU:HD13	1:136:A:SER:H	19	0.38	0.13	0.36
(2,1626)	1:139:A:LEU:HD12	1:136:A:SER:H	19	0.38	0.13	0.36
(2,1626)	1:135:A:LEU:HD21	1:136:A:SER:H	19	0.38	0.13	0.36
(2,1626)	1:135:A:LEU:HD12	1:136:A:SER:H	19	0.38	0.13	0.36
(2,1626)	1:135:A:LEU:HD23	1:136:A:SER:H	19	0.38	0.13	0.36
(2,885)	1:66:A:ILE:HD11	1:26:A:ASP:H	19	0.34	0.13	0.29
(2,885)	1:66:A:ILE:HD12	1:26:A:ASP:H	19	0.34	0.13	0.29
(2,885)	1:66:A:ILE:HD13	1:26:A:ASP:H	19	0.34	0.13	0.29
(2,882)	1:28:A:LEU:HD21	1:28:A:LEU:H	19	0.3	0.08	0.29
(2,882)	1:28:A:LEU:HD22	1:28:A:LEU:H	19	0.3	0.08	0.29
(2,882)	1:28:A:LEU:HD23	1:28:A:LEU:H	19	0.3	0.08	0.29
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	19	0.3	0.06	0.31
(2,4474)	1:36:A:LEU:HD23	1:41:A:TYR:HD1	19	0.3	0.19	0.23
(2,4474)	1:36:A:LEU:HD21	1:41:A:TYR:HD1	19	0.3	0.19	0.23
(2,4474)	1:36:A:LEU:HD22	1:41:A:TYR:HD1	19	0.3	0.19	0.23
(2,4474)	1:36:A:LEU:HD22	1:41:A:TYR:HD2	19	0.3	0.19	0.23
(2,4474)	1:36:A:LEU:HD23	1:41:A:TYR:HD2	19	0.3	0.19	0.23
(2,4474)	1:36:A:LEU:HD21	1:41:A:TYR:HD2	19	0.3	0.19	0.23
(2,4474)	1:36:A:LEU:HD23	1:21:A:TYR:HD1	19	0.3	0.19	0.23
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	19	0.29	0.03	0.29
(2,1248)	1:94:A:LEU:HD13	1:95:A:LEU:H	19	0.29	0.08	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1248)	1:94:A:LEU:HD11	1:95:A:LEU:H	19	0.29	0.08	0.28
(2,1248)	1:94:A:LEU:HD12	1:95:A:LEU:H	19	0.29	0.08	0.28
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG11	19	0.28	0.09	0.3
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG13	19	0.28	0.09	0.3
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG12	19	0.28	0.09	0.3
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG21	19	0.28	0.1	0.29
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG22	19	0.28	0.1	0.29
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG23	19	0.28	0.1	0.29
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	19	0.27	0.11	0.25
(2,1019)	1:67:A:PRO:HB3	1:66:A:ILE:H	19	0.27	0.11	0.25
(2,2658)	1:81:A:VAL:HG22	1:79:A:TYR:HB2	19	0.26	0.07	0.26
(2,2658)	1:81:A:VAL:HG21	1:79:A:TYR:HB2	19	0.26	0.07	0.26
(2,2658)	1:81:A:VAL:HG23	1:79:A:TYR:HB2	19	0.26	0.07	0.26
(2,1082)	1:24:A:ILE:HG23	1:25:A:LYS:H	19	0.24	0.06	0.22
(2,1082)	1:24:A:ILE:HG22	1:25:A:LYS:H	19	0.24	0.06	0.22
(2,1082)	1:24:A:ILE:HG21	1:25:A:LYS:H	19	0.24	0.06	0.22
(2,597)	1:52:A:LEU:HD11	1:52:A:LEU:H	19	0.24	0.03	0.24
(2,597)	1:52:A:LEU:HD23	1:52:A:LEU:H	19	0.24	0.03	0.24
(2,597)	1:52:A:LEU:HD12	1:52:A:LEU:H	19	0.24	0.03	0.24
(2,597)	1:52:A:LEU:HD13	1:52:A:LEU:H	19	0.24	0.03	0.24
(2,597)	1:52:A:LEU:HD22	1:52:A:LEU:H	19	0.24	0.03	0.24
(2,597)	1:52:A:LEU:HD21	1:52:A:LEU:H	19	0.24	0.03	0.24
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD11	19	0.24	0.03	0.24
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD23	19	0.24	0.03	0.24
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD12	19	0.24	0.03	0.24
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD13	19	0.24	0.03	0.24
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD22	19	0.24	0.03	0.24
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD21	19	0.24	0.03	0.24
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	19	0.22	0.06	0.2
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	19	0.2	0.04	0.2
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG22	19	0.2	0.08	0.17
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG23	19	0.2	0.08	0.17
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG21	19	0.2	0.08	0.17
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	19	0.2	0.04	0.19
(2,1179)	1:35:A:ARG:HD3	1:20:A:GLU:H	19	0.2	0.04	0.19
(2,1401)	1:106:A:VAL:HG22	1:105:A:ASN:HD22	18	0.93	0.43	0.97
(2,1401)	1:106:A:VAL:HG23	1:105:A:ASN:HD22	18	0.93	0.43	0.97
(2,1401)	1:106:A:VAL:HG21	1:105:A:ASN:HD22	18	0.93	0.43	0.97
(2,1401)	1:106:A:VAL:HG12	1:105:A:ASN:HD22	18	0.93	0.43	0.97
(2,1401)	1:106:A:VAL:HG11	1:105:A:ASN:HD22	18	0.93	0.43	0.97
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG22	18	0.62	0.19	0.66
(2,3361)	1:60:A:LEU:H	1:64:A:VAL:HG22	18	0.62	0.19	0.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3361)	1:87:A:ASN:HD22	1:64:A:VAL:HG23	18	0.62	0.19	0.66
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG21	18	0.62	0.19	0.66
(2,3361)	1:87:A:ASN:HD22	1:64:A:VAL:HG22	18	0.62	0.19	0.66
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG23	18	0.62	0.19	0.66
(2,3361)	1:87:A:ASN:HD22	1:64:A:VAL:HG21	18	0.62	0.19	0.66
(2,4243)	1:102:A:VAL:HG23	1:104:A:LEU:HA	18	0.5	0.25	0.46
(2,4243)	1:102:A:VAL:HG22	1:104:A:LEU:HA	18	0.5	0.25	0.46
(2,4243)	1:102:A:VAL:HG21	1:104:A:LEU:HA	18	0.5	0.25	0.46
(2,4551)	1:34:A:ILE:HG23	1:120:A:PHE:HE2	18	0.49	0.19	0.53
(2,4551)	1:122:A:ILE:HD13	1:120:A:PHE:HE2	18	0.49	0.19	0.53
(2,4551)	1:122:A:ILE:HD11	1:120:A:PHE:HE1	18	0.49	0.19	0.53
(2,4551)	1:122:A:ILE:HD12	1:120:A:PHE:HE2	18	0.49	0.19	0.53
(2,4551)	1:69:A:ILE:HD12	1:120:A:PHE:HE2	18	0.49	0.19	0.53
(2,4551)	1:69:A:ILE:HD12	1:120:A:PHE:HE1	18	0.49	0.19	0.53
(2,4551)	1:69:A:ILE:HD13	1:120:A:PHE:HE1	18	0.49	0.19	0.53
(2,4551)	1:34:A:ILE:HG22	1:120:A:PHE:HE2	18	0.49	0.19	0.53
(2,4551)	1:122:A:ILE:HD12	1:120:A:PHE:HE1	18	0.49	0.19	0.53
(2,4551)	1:69:A:ILE:HD13	1:120:A:PHE:HE2	18	0.49	0.19	0.53
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD12	18	0.47	0.15	0.44
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD11	18	0.47	0.15	0.44
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD13	18	0.47	0.15	0.44
(2,4334)	1:120:A:PHE:HB2	1:122:A:ILE:HD12	18	0.47	0.15	0.44
(2,760)	1:41:A:TYR:HB2	1:34:A:ILE:H	18	0.38	0.15	0.38
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	18	0.38	0.15	0.38
(2,760)	1:33:A:LYS:HE3	1:34:A:ILE:H	18	0.38	0.15	0.38
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD1	18	0.36	0.17	0.32
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD2	18	0.36	0.17	0.32
(2,3836)	1:31:A:LYS:HD2	1:22:A:VAL:HG11	18	0.34	0.12	0.34
(2,3836)	1:90:A:ALA:HB3	1:64:A:VAL:HG12	18	0.34	0.12	0.34
(2,3836)	1:90:A:ALA:HB2	1:64:A:VAL:HG12	18	0.34	0.12	0.34
(2,3836)	1:90:A:ALA:HB1	1:64:A:VAL:HG13	18	0.34	0.12	0.34
(2,3836)	1:90:A:ALA:HB1	1:64:A:VAL:HG12	18	0.34	0.12	0.34
(2,3836)	1:90:A:ALA:HB1	1:64:A:VAL:HG11	18	0.34	0.12	0.34
(2,3836)	1:90:A:ALA:HB2	1:64:A:VAL:HG11	18	0.34	0.12	0.34
(2,3836)	1:90:A:ALA:HB3	1:64:A:VAL:HG11	18	0.34	0.12	0.34
(2,3836)	1:90:A:ALA:HB3	1:64:A:VAL:HG13	18	0.34	0.12	0.34
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	18	0.34	0.07	0.34
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	18	0.34	0.07	0.34
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	18	0.34	0.07	0.34
(2,877)	1:60:A:LEU:HD21	1:86:A:TRP:H	18	0.32	0.1	0.3
(2,877)	1:60:A:LEU:HD22	1:86:A:TRP:H	18	0.32	0.1	0.3
(2,877)	1:60:A:LEU:HD23	1:86:A:TRP:H	18	0.32	0.1	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,877)	1:63:A:LEU:HB2	1:86:A:TRP:H	18	0.32	0.1	0.3
(2,841)	1:5:A:ILE:HD12	1:5:A:ILE:H	18	0.32	0.12	0.34
(2,841)	1:139:A:LEU:HD21	1:139:A:LEU:H	18	0.32	0.12	0.34
(2,841)	1:139:A:LEU:HD23	1:139:A:LEU:H	18	0.32	0.12	0.34
(2,841)	1:139:A:LEU:HD22	1:139:A:LEU:H	18	0.32	0.12	0.34
(2,841)	1:5:A:ILE:HD11	1:5:A:ILE:H	18	0.32	0.12	0.34
(2,841)	1:5:A:ILE:HD13	1:5:A:ILE:H	18	0.32	0.12	0.34
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	18	0.29	0.11	0.26
(2,895)	1:91:A:ILE:HD13	1:88:A:LYS:H	18	0.29	0.09	0.29
(2,895)	1:91:A:ILE:HD12	1:88:A:LYS:H	18	0.29	0.09	0.29
(2,895)	1:91:A:ILE:HD11	1:88:A:LYS:H	18	0.29	0.09	0.29
(2,1509)	1:63:A:LEU:HA	1:62:A:SER:H	18	0.28	0.06	0.29
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	18	0.28	0.06	0.29
(2,80)	1:34:A:ILE:HG22	1:35:A:ARG:H	18	0.24	0.07	0.22
(2,80)	1:34:A:ILE:HG21	1:35:A:ARG:H	18	0.24	0.07	0.22
(2,80)	1:34:A:ILE:HG23	1:35:A:ARG:H	18	0.24	0.07	0.22
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD11	18	0.23	0.06	0.25
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	18	0.23	0.06	0.25
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD13	18	0.23	0.06	0.25
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	18	0.23	0.08	0.21
(2,1104)	1:37:A:ASN:H	1:20:A:GLU:H	18	0.23	0.08	0.21
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	18	0.22	0.05	0.24
(2,910)	1:27:A:ALA:H	1:29:A:ASP:H	18	0.22	0.05	0.24
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	18	0.21	0.05	0.2
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	18	0.2	0.04	0.19
(2,3467)	1:52:A:LEU:HA	1:51:A:LYS:HG3	18	0.2	0.04	0.19
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG3	18	0.2	0.04	0.19
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE1	18	0.19	0.03	0.18
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE2	18	0.19	0.03	0.18
(2,4659)	1:21:A:TYR:HB3	1:21:A:TYR:HE2	18	0.19	0.03	0.18
(2,4659)	1:21:A:TYR:HB3	1:21:A:TYR:HE1	18	0.19	0.03	0.18
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	18	0.19	0.05	0.17
(2,4225)	1:23:A:THR:HG22	1:62:A:SER:HB2	18	0.18	0.02	0.18
(2,4225)	1:23:A:THR:HG23	1:62:A:SER:HB2	18	0.18	0.02	0.18
(2,4225)	1:23:A:THR:HG21	1:62:A:SER:HB2	18	0.18	0.02	0.18
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	18	0.16	0.02	0.16
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	18	0.15	0.04	0.13
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	18	0.13	0.01	0.13
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB1	17	0.91	0.57	1.24
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB3	17	0.91	0.57	1.24
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB2	17	0.91	0.57	1.24
(2,4093)	1:120:A:PHE:HD1	1:122:A:ILE:HD13	17	0.59	0.23	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4093)	1:120:A:PHE:HD1	1:122:A:ILE:HD11	17	0.59	0.23	0.58
(2,4093)	1:120:A:PHE:HD2	1:122:A:ILE:HD12	17	0.59	0.23	0.58
(2,4093)	1:120:A:PHE:HD1	1:69:A:ILE:HD12	17	0.59	0.23	0.58
(2,4093)	1:120:A:PHE:HD1	1:122:A:ILE:HD12	17	0.59	0.23	0.58
(2,4093)	1:120:A:PHE:HD2	1:122:A:ILE:HD13	17	0.59	0.23	0.58
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB3	17	0.47	0.27	0.38
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB1	17	0.47	0.27	0.38
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB2	17	0.47	0.27	0.38
(2,4318)	1:31:A:LYS:HB3	1:27:A:ALA:HB2	17	0.47	0.27	0.38
(2,4318)	1:31:A:LYS:HB3	1:27:A:ALA:HB3	17	0.47	0.27	0.38
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD2	17	0.47	0.2	0.49
(2,4438)	1:35:A:ARG:HD3	1:41:A:TYR:HD1	17	0.47	0.2	0.49
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD1	17	0.47	0.2	0.49
(2,4438)	1:35:A:ARG:HD3	1:41:A:TYR:HD2	17	0.47	0.2	0.49
(2,4373)	1:133:A:THR:HG22	1:137:A:GLU:HB3	17	0.46	0.14	0.44
(2,4373)	1:130:A:THR:HG21	1:134:A:GLU:HB3	17	0.46	0.14	0.44
(2,4373)	1:133:A:THR:HG23	1:137:A:GLU:HB3	17	0.46	0.14	0.44
(2,4373)	1:130:A:THR:HG23	1:131:A:GLU:HB2	17	0.46	0.14	0.44
(2,4373)	1:130:A:THR:HG22	1:134:A:GLU:HB3	17	0.46	0.14	0.44
(2,4373)	1:130:A:THR:HG21	1:131:A:GLU:HB3	17	0.46	0.14	0.44
(2,4373)	1:130:A:THR:HG23	1:134:A:GLU:HB3	17	0.46	0.14	0.44
(2,4373)	1:133:A:THR:HG21	1:137:A:GLU:HB3	17	0.46	0.14	0.44
(2,4373)	1:130:A:THR:HG22	1:131:A:GLU:HB3	17	0.46	0.14	0.44
(2,2542)	1:115:A:TYR:HD1	1:111:A:LEU:HB2	17	0.42	0.16	0.41
(2,2542)	1:115:A:TYR:HD2	1:111:A:LEU:HB2	17	0.42	0.16	0.41
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE1	17	0.41	0.18	0.42
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE2	17	0.41	0.18	0.42
(2,2175)	1:94:A:LEU:HD23	1:52:A:LEU:HA	17	0.4	0.14	0.43
(2,2175)	1:94:A:LEU:HD22	1:52:A:LEU:HA	17	0.4	0.14	0.43
(2,2175)	1:94:A:LEU:HD21	1:52:A:LEU:HA	17	0.4	0.14	0.43
(2,2473)	1:69:A:ILE:HD13	1:18:A:PRO:HD3	17	0.37	0.14	0.42
(2,2473)	1:69:A:ILE:HD12	1:18:A:PRO:HD3	17	0.37	0.14	0.42
(2,2473)	1:122:A:ILE:HD11	1:18:A:PRO:HD3	17	0.37	0.14	0.42
(2,2473)	1:69:A:ILE:HD11	1:18:A:PRO:HD3	17	0.37	0.14	0.42
(2,2473)	1:122:A:ILE:HD12	1:18:A:PRO:HD3	17	0.37	0.14	0.42
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD13	17	0.37	0.14	0.42
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD12	17	0.37	0.14	0.42
(2,4333)	1:18:A:PRO:HD3	1:122:A:ILE:HD11	17	0.37	0.14	0.42
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD11	17	0.37	0.14	0.42
(2,4333)	1:18:A:PRO:HD3	1:122:A:ILE:HD12	17	0.37	0.14	0.42
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG21	17	0.37	0.14	0.36
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG23	17	0.37	0.14	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG22	17	0.37	0.14	0.36
(2,348)	1:58:A:LEU:HD23	1:61:A:TRP:H	17	0.33	0.18	0.32
(2,348)	1:58:A:LEU:HD21	1:61:A:TRP:H	17	0.33	0.18	0.32
(2,348)	1:58:A:LEU:HD22	1:61:A:TRP:H	17	0.33	0.18	0.32
(2,348)	1:24:A:ILE:HG22	1:61:A:TRP:H	17	0.33	0.18	0.32
(2,2143)	1:130:A:THR:HG21	1:131:A:GLU:HA	17	0.32	0.14	0.31
(2,2143)	1:133:A:THR:HG22	1:134:A:GLU:HA	17	0.32	0.14	0.31
(2,2143)	1:133:A:THR:HG21	1:134:A:GLU:HA	17	0.32	0.14	0.31
(2,2143)	1:133:A:THR:HG23	1:134:A:GLU:HA	17	0.32	0.14	0.31
(2,33)	1:46:A:LYS:HD3	1:46:A:LYS:H	17	0.32	0.13	0.29
(2,33)	1:46:A:LYS:HD2	1:46:A:LYS:H	17	0.32	0.13	0.29
(2,33)	1:45:A:LYS:HD2	1:46:A:LYS:H	17	0.32	0.13	0.29
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	17	0.32	0.19	0.27
(2,1499)	1:93:A:ILE:HG23	1:96:A:GLY:H	17	0.31	0.14	0.29
(2,1499)	1:93:A:ILE:HG22	1:96:A:GLY:H	17	0.31	0.14	0.29
(2,1499)	1:93:A:ILE:HG21	1:96:A:GLY:H	17	0.31	0.14	0.29
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	17	0.3	0.17	0.24
(2,516)	1:72:A:LYS:HD2	1:80:A:PHE:H	17	0.3	0.17	0.24
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE1	17	0.29	0.1	0.26
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE2	17	0.29	0.1	0.26
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG23	17	0.27	0.08	0.28
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG22	17	0.27	0.08	0.28
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG21	17	0.27	0.08	0.28
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD12	17	0.26	0.12	0.2
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD11	17	0.26	0.12	0.2
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD13	17	0.26	0.12	0.2
(2,831)	1:119:A:ILE:HD12	1:112:A:LEU:H	17	0.26	0.1	0.26
(2,831)	1:119:A:ILE:HD11	1:112:A:LEU:H	17	0.26	0.1	0.26
(2,831)	1:112:A:LEU:HD21	1:112:A:LEU:H	17	0.26	0.1	0.26
(2,831)	1:112:A:LEU:HD13	1:112:A:LEU:H	17	0.26	0.1	0.26
(2,831)	1:119:A:ILE:HD13	1:112:A:LEU:H	17	0.26	0.1	0.26
(2,831)	1:112:A:LEU:HD11	1:112:A:LEU:H	17	0.26	0.1	0.26
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG11	17	0.25	0.1	0.25
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG13	17	0.25	0.1	0.25
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG12	17	0.25	0.1	0.25
(2,3672)	1:79:A:TYR:H	1:102:A:VAL:HG11	17	0.25	0.1	0.25
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD12	17	0.24	0.04	0.24
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD13	17	0.24	0.04	0.24
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD11	17	0.24	0.04	0.24
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	17	0.24	0.05	0.25
(2,4020)	1:118:A:LEU:HB3	1:44:A:ILE:HG23	17	0.24	0.07	0.24
(2,4020)	1:49:A:VAL:HB	1:44:A:ILE:HG23	17	0.24	0.07	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4020)	1:49:A:VAL:HB	1:44:A:ILE:HG21	17	0.24	0.07	0.24
(2,4020)	1:118:A:LEU:HB3	1:44:A:ILE:HG22	17	0.24	0.07	0.24
(2,4020)	1:49:A:VAL:HB	1:44:A:ILE:HG22	17	0.24	0.07	0.24
(2,4020)	1:118:A:LEU:HB3	1:44:A:ILE:HG21	17	0.24	0.07	0.24
(2,4020)	1:67:A:PRO:HB3	1:44:A:ILE:HG23	17	0.24	0.07	0.24
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	17	0.23	0.05	0.22
(2,605)	1:28:A:LEU:HD23	1:51:A:LYS:H	17	0.23	0.09	0.21
(2,605)	1:28:A:LEU:HD21	1:51:A:LYS:H	17	0.23	0.09	0.21
(2,605)	1:28:A:LEU:HD22	1:51:A:LYS:H	17	0.23	0.09	0.21
(2,154)	1:71:A:ILE:HD13	1:122:A:ILE:H	17	0.23	0.08	0.21
(2,154)	1:71:A:ILE:HD11	1:122:A:ILE:H	17	0.23	0.08	0.21
(2,154)	1:71:A:ILE:HD12	1:122:A:ILE:H	17	0.23	0.08	0.21
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	17	0.22	0.06	0.21
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	16	0.47	0.14	0.49
(2,3347)	1:120:A:PHE:HD1	1:69:A:ILE:HG12	16	0.47	0.14	0.49
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG22	16	0.45	0.16	0.44
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG23	16	0.45	0.16	0.44
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG21	16	0.45	0.16	0.44
(2,4310)	1:120:A:PHE:HD2	1:69:A:ILE:HG23	16	0.45	0.16	0.44
(2,4310)	1:120:A:PHE:HD2	1:69:A:ILE:HG21	16	0.45	0.16	0.44
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	16	0.41	0.08	0.42
(2,1874)	1:69:A:ILE:HG13	1:82:A:SER:HB3	16	0.41	0.08	0.42
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	16	0.41	0.04	0.4
(2,4223)	1:71:A:ILE:HG13	1:82:A:SER:HB2	16	0.41	0.04	0.4
(2,663)	1:115:A:TYR:HD1	1:112:A:LEU:H	16	0.33	0.12	0.34
(2,663)	1:115:A:TYR:HD2	1:112:A:LEU:H	16	0.33	0.12	0.34
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG21	16	0.31	0.12	0.28
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG23	16	0.31	0.12	0.28
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG22	16	0.31	0.12	0.28
(2,1255)	1:52:A:LEU:HD11	1:54:A:SER:H	16	0.3	0.12	0.26
(2,1255)	1:28:A:LEU:HD23	1:54:A:SER:H	16	0.3	0.12	0.26
(2,1255)	1:52:A:LEU:HD12	1:54:A:SER:H	16	0.3	0.12	0.26
(2,1255)	1:28:A:LEU:HD22	1:54:A:SER:H	16	0.3	0.12	0.26
(2,1255)	1:52:A:LEU:HD13	1:54:A:SER:H	16	0.3	0.12	0.26
(2,1255)	1:28:A:LEU:HD21	1:54:A:SER:H	16	0.3	0.12	0.26
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD11	16	0.29	0.09	0.3
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD12	16	0.29	0.09	0.3
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD13	16	0.29	0.09	0.3
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	16	0.29	0.09	0.3
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	16	0.29	0.09	0.3
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	16	0.29	0.09	0.3
(2,1781)	1:68:A:PHE:HE2	1:91:A:ILE:HA	16	0.26	0.1	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1781)	1:68:A:PHE:HE1	1:91:A:ILE:HA	16	0.26	0.1	0.28
(2,3471)	1:118:A:LEU:HA	1:44:A:ILE:HG12	16	0.25	0.09	0.22
(2,3471)	1:32:A:LEU:HA	1:44:A:ILE:HG13	16	0.25	0.09	0.22
(2,4207)	1:70:A:PHE:HE1	1:91:A:ILE:HD12	16	0.2	0.08	0.18
(2,4207)	1:70:A:PHE:HE2	1:91:A:ILE:HD11	16	0.2	0.08	0.18
(2,4207)	1:70:A:PHE:HE1	1:91:A:ILE:HD11	16	0.2	0.08	0.18
(2,4207)	1:68:A:PHE:HE2	1:91:A:ILE:HD11	16	0.2	0.08	0.18
(2,4207)	1:68:A:PHE:HE2	1:91:A:ILE:HD13	16	0.2	0.08	0.18
(2,4207)	1:70:A:PHE:HE2	1:91:A:ILE:HD13	16	0.2	0.08	0.18
(2,4207)	1:68:A:PHE:HE1	1:91:A:ILE:HD11	16	0.2	0.08	0.18
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	16	0.19	0.04	0.2
(2,862)	1:111:A:LEU:HD23	1:111:A:LEU:H	16	0.17	0.03	0.18
(2,862)	1:95:A:LEU:HD21	1:111:A:LEU:H	16	0.17	0.03	0.18
(2,862)	1:111:A:LEU:HD21	1:111:A:LEU:H	16	0.17	0.03	0.18
(2,862)	1:95:A:LEU:HD23	1:111:A:LEU:H	16	0.17	0.03	0.18
(2,862)	1:111:A:LEU:HD22	1:111:A:LEU:H	16	0.17	0.03	0.18
(2,862)	1:95:A:LEU:HD22	1:111:A:LEU:H	16	0.17	0.03	0.18
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	16	0.16	0.04	0.17
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	16	0.14	0.02	0.15
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	16	0.12	0.01	0.12
(2,4660)	1:41:A:TYR:HB2	1:41:A:TYR:HE2	16	0.12	0.01	0.12
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE1	16	0.12	0.01	0.12
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE2	16	0.12	0.01	0.12
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	15	0.77	0.29	0.98
(2,1556)	1:44:A:ILE:HB	1:43:A:GLU:H	15	0.77	0.29	0.98
(2,1556)	1:33:A:LYS:HB3	1:43:A:GLU:H	15	0.77	0.29	0.98
(2,4300)	1:65:A:LYS:HE3	1:63:A:LEU:HD23	15	0.74	0.25	0.7
(2,4300)	1:65:A:LYS:HE2	1:63:A:LEU:HD22	15	0.74	0.25	0.7
(2,4300)	1:59:A:TYR:HB2	1:63:A:LEU:HD21	15	0.74	0.25	0.7
(2,4300)	1:65:A:LYS:HE3	1:63:A:LEU:HD22	15	0.74	0.25	0.7
(2,4300)	1:59:A:TYR:HB2	1:63:A:LEU:HD23	15	0.74	0.25	0.7
(2,4300)	1:65:A:LYS:HE3	1:63:A:LEU:HD21	15	0.74	0.25	0.7
(2,4300)	1:65:A:LYS:HE2	1:63:A:LEU:HD23	15	0.74	0.25	0.7
(2,4689)	1:123:A:LEU:HD21	1:79:A:TYR:HD1	15	0.57	0.25	0.56
(2,4689)	1:123:A:LEU:HD23	1:79:A:TYR:HD1	15	0.57	0.25	0.56
(2,4689)	1:72:A:LYS:HG2	1:79:A:TYR:HD2	15	0.57	0.25	0.56
(2,4689)	1:123:A:LEU:HD22	1:79:A:TYR:HD2	15	0.57	0.25	0.56
(2,4689)	1:123:A:LEU:HD21	1:79:A:TYR:HD2	15	0.57	0.25	0.56
(2,4689)	1:123:A:LEU:HD22	1:79:A:TYR:HD1	15	0.57	0.25	0.56
(2,4689)	1:123:A:LEU:HD23	1:79:A:TYR:HD2	15	0.57	0.25	0.56
(2,2560)	1:21:A:TYR:HE1	1:34:A:ILE:HB	15	0.44	0.16	0.45
(2,2560)	1:42:A:HIS:HD2	1:34:A:ILE:HB	15	0.44	0.16	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2560)	1:120:A:PHE:HE1	1:34:A:ILE:HB	15	0.44	0.16	0.45
(2,2560)	1:120:A:PHE:HE2	1:34:A:ILE:HB	15	0.44	0.16	0.45
(2,2560)	1:21:A:TYR:HE2	1:34:A:ILE:HB	15	0.44	0.16	0.45
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	15	0.39	0.01	0.4
(2,2375)	1:104:A:LEU:HD22	1:78:A:GLU:HA	15	0.38	0.2	0.3
(2,2375)	1:104:A:LEU:HD23	1:78:A:GLU:HA	15	0.38	0.2	0.3
(2,2375)	1:104:A:LEU:HD21	1:78:A:GLU:HA	15	0.38	0.2	0.3
(2,2375)	1:118:A:LEU:HD11	1:115:A:TYR:HA	15	0.38	0.2	0.3
(2,2375)	1:118:A:LEU:HD12	1:115:A:TYR:HA	15	0.38	0.2	0.3
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	15	0.36	0.13	0.37
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	15	0.34	0.11	0.3
(2,1877)	1:137:A:GLU:HB2	1:136:A:SER:HB2	15	0.33	0.13	0.35
(2,1877)	1:135:A:LEU:HB3	1:136:A:SER:HB3	15	0.33	0.13	0.35
(2,1877)	1:135:A:LEU:HB2	1:136:A:SER:HB2	15	0.33	0.13	0.35
(2,1877)	1:90:A:ALA:HB3	1:64:A:VAL:HA	15	0.33	0.13	0.35
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG21	15	0.32	0.14	0.31
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG23	15	0.32	0.14	0.31
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG22	15	0.32	0.14	0.31
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD13	15	0.27	0.15	0.22
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD12	15	0.27	0.15	0.22
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD11	15	0.27	0.15	0.22
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD11	15	0.25	0.09	0.23
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD13	15	0.25	0.09	0.23
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD12	15	0.25	0.09	0.23
(2,3389)	1:41:A:TYR:HD1	1:36:A:LEU:HG	15	0.22	0.12	0.17
(2,3389)	1:41:A:TYR:HD2	1:36:A:LEU:HG	15	0.22	0.12	0.17
(2,3389)	1:21:A:TYR:HD1	1:69:A:ILE:HG13	15	0.22	0.12	0.17
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	15	0.17	0.06	0.16
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	15	0.12	0.01	0.12
(2,2338)	1:67:A:PRO:HG3	1:21:A:TYR:HA	14	0.68	0.35	0.68
(2,2338)	1:65:A:LYS:HD3	1:21:A:TYR:HA	14	0.68	0.35	0.68
(2,2338)	1:72:A:LYS:HD3	1:79:A:TYR:HA	14	0.68	0.35	0.68
(2,2338)	1:65:A:LYS:HD2	1:21:A:TYR:HA	14	0.68	0.35	0.68
(2,1660)	1:130:A:THR:HG21	1:132:A:GLU:H	14	0.37	0.19	0.3
(2,1660)	1:130:A:THR:HG22	1:132:A:GLU:H	14	0.37	0.19	0.3
(2,1660)	1:130:A:THR:HG23	1:132:A:GLU:H	14	0.37	0.19	0.3
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	14	0.33	0.11	0.34
(2,67)	1:33:A:LYS:HE2	1:43:A:GLU:H	14	0.33	0.11	0.34
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE1	14	0.32	0.13	0.36
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE2	14	0.32	0.13	0.36
(2,4669)	1:18:A:PRO:HG3	1:21:A:TYR:HE2	14	0.32	0.13	0.36
(2,160)	1:121:A:ILE:HG21	1:70:A:PHE:H	14	0.3	0.1	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,160)	1:121:A:ILE:HG23	1:70:A:PHE:H	14	0.3	0.1	0.3
(2,160)	1:121:A:ILE:HG22	1:70:A:PHE:H	14	0.3	0.1	0.3
(2,160)	1:71:A:ILE:HG12	1:70:A:PHE:H	14	0.3	0.1	0.3
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	14	0.28	0.12	0.26
(2,2844)	1:51:A:LYS:HG3	1:47:A:ASP:HB3	14	0.28	0.12	0.26
(2,2844)	1:51:A:LYS:HD2	1:47:A:ASP:HB3	14	0.28	0.12	0.26
(2,2538)	1:115:A:TYR:HD2	1:118:A:LEU:HB3	14	0.27	0.11	0.24
(2,2538)	1:115:A:TYR:HD1	1:118:A:LEU:HB3	14	0.27	0.11	0.24
(2,1891)	1:63:A:LEU:HD23	1:62:A:SER:HB3	14	0.24	0.05	0.22
(2,1891)	1:63:A:LEU:HD22	1:62:A:SER:HB3	14	0.24	0.05	0.22
(2,1891)	1:63:A:LEU:HD21	1:62:A:SER:HB3	14	0.24	0.05	0.22
(2,84)	1:24:A:ILE:HG23	1:61:A:TRP:HE1	14	0.2	0.07	0.18
(2,84)	1:24:A:ILE:HG21	1:61:A:TRP:HE1	14	0.2	0.07	0.18
(2,84)	1:24:A:ILE:HG22	1:61:A:TRP:HE1	14	0.2	0.07	0.18
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD11	14	0.18	0.04	0.19
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD12	14	0.18	0.04	0.19
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD13	14	0.18	0.04	0.19
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	14	0.17	0.05	0.18
(2,492)	1:105:A:ASN:HB3	1:79:A:TYR:H	14	0.17	0.05	0.18
(2,492)	1:105:A:ASN:HB2	1:79:A:TYR:H	14	0.17	0.05	0.18
(2,871)	1:119:A:ILE:HD11	1:119:A:ILE:H	14	0.16	0.04	0.16
(2,871)	1:119:A:ILE:HD13	1:119:A:ILE:H	14	0.16	0.04	0.16
(2,871)	1:119:A:ILE:HD12	1:119:A:ILE:H	14	0.16	0.04	0.16
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	14	0.14	0.02	0.14
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	14	0.14	0.02	0.14
(2,2865)	1:104:A:LEU:HD23	1:105:A:ASN:HB3	13	0.39	0.24	0.34
(2,2865)	1:76:A:ILE:HG23	1:105:A:ASN:HB2	13	0.39	0.24	0.34
(2,2865)	1:76:A:ILE:HG21	1:105:A:ASN:HB2	13	0.39	0.24	0.34
(2,2865)	1:104:A:LEU:HD21	1:105:A:ASN:HB3	13	0.39	0.24	0.34
(2,2865)	1:104:A:LEU:HD22	1:105:A:ASN:HB3	13	0.39	0.24	0.34
(2,2865)	1:76:A:ILE:HG22	1:105:A:ASN:HB2	13	0.39	0.24	0.34
(2,2496)	1:46:A:LYS:HG3	1:30:A:GLY:HA2	13	0.34	0.16	0.32
(2,2496)	1:32:A:LEU:HB2	1:30:A:GLY:HA2	13	0.34	0.16	0.32
(2,2490)	1:31:A:LYS:HG3	1:30:A:GLY:HA3	13	0.29	0.1	0.34
(2,2490)	1:31:A:LYS:HG2	1:30:A:GLY:HA3	13	0.29	0.1	0.34
(2,4465)	1:118:A:LEU:HD11	1:115:A:TYR:HD2	13	0.28	0.15	0.24
(2,4465)	1:118:A:LEU:HD11	1:115:A:TYR:HD1	13	0.28	0.15	0.24
(2,4465)	1:118:A:LEU:HD13	1:115:A:TYR:HD2	13	0.28	0.15	0.24
(2,4465)	1:118:A:LEU:HD12	1:115:A:TYR:HD1	13	0.28	0.15	0.24
(2,4465)	1:118:A:LEU:HD12	1:115:A:TYR:HD2	13	0.28	0.15	0.24
(2,4465)	1:118:A:LEU:HD13	1:115:A:TYR:HD1	13	0.28	0.15	0.24
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	13	0.27	0.06	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1388)	1:22:A:VAL:HG13	1:21:A:TYR:H	13	0.24	0.09	0.25
(2,1388)	1:34:A:ILE:HG21	1:21:A:TYR:H	13	0.24	0.09	0.25
(2,1388)	1:34:A:ILE:HG22	1:21:A:TYR:H	13	0.24	0.09	0.25
(2,1388)	1:22:A:VAL:HG12	1:21:A:TYR:H	13	0.24	0.09	0.25
(2,1388)	1:22:A:VAL:HG11	1:21:A:TYR:H	13	0.24	0.09	0.25
(2,1388)	1:34:A:ILE:HG23	1:21:A:TYR:H	13	0.24	0.09	0.25
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	13	0.23	0.1	0.23
(2,1998)	1:115:A:TYR:HD1	1:112:A:LEU:HA	13	0.23	0.09	0.18
(2,1998)	1:115:A:TYR:HD2	1:112:A:LEU:HA	13	0.23	0.09	0.18
(2,2827)	1:45:A:LYS:HB3	1:47:A:ASP:HB3	13	0.21	0.07	0.23
(2,2827)	1:50:A:GLU:HB2	1:47:A:ASP:HB3	13	0.21	0.07	0.23
(2,571)	1:118:A:LEU:HD12	1:52:A:LEU:H	13	0.2	0.06	0.19
(2,571)	1:118:A:LEU:HD11	1:52:A:LEU:H	13	0.2	0.06	0.19
(2,571)	1:118:A:LEU:HD13	1:52:A:LEU:H	13	0.2	0.06	0.19
(2,95)	1:70:A:PHE:HD2	1:122:A:ILE:H	13	0.19	0.07	0.19
(2,95)	1:70:A:PHE:HD1	1:122:A:ILE:H	13	0.19	0.07	0.19
(2,3632)	1:94:A:LEU:HD13	1:95:A:LEU:HG	13	0.18	0.05	0.18
(2,3632)	1:94:A:LEU:HD11	1:95:A:LEU:HG	13	0.18	0.05	0.18
(2,3632)	1:94:A:LEU:HD12	1:95:A:LEU:HG	13	0.18	0.05	0.18
(2,3632)	1:103:A:ILE:HG23	1:95:A:LEU:HG	13	0.18	0.05	0.18
(2,2179)	1:108:A:VAL:HG13	1:105:A:ASN:HA	13	0.17	0.06	0.16
(2,2179)	1:108:A:VAL:HG12	1:105:A:ASN:HA	13	0.17	0.06	0.16
(2,2179)	1:108:A:VAL:HG11	1:105:A:ASN:HA	13	0.17	0.06	0.16
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	13	0.11	0.01	0.11
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	13	0.11	0.01	0.11
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	13	0.11	0.01	0.11
(2,1885)	1:123:A:LEU:HD21	1:125:A:PRO:HA	12	0.82	0.19	0.77
(2,1885)	1:123:A:LEU:HD22	1:125:A:PRO:HA	12	0.82	0.19	0.77
(2,1885)	1:123:A:LEU:HD23	1:125:A:PRO:HA	12	0.82	0.19	0.77
(2,1885)	1:122:A:ILE:HG21	1:125:A:PRO:HA	12	0.82	0.19	0.77
(2,1885)	1:122:A:ILE:HG22	1:125:A:PRO:HA	12	0.82	0.19	0.77
(2,2652)	1:95:A:LEU:HD23	1:107:A:ASP:HB2	12	0.78	0.28	0.84
(2,2652)	1:95:A:LEU:HD22	1:107:A:ASP:HB2	12	0.78	0.28	0.84
(2,2652)	1:104:A:LEU:HD23	1:107:A:ASP:HB2	12	0.78	0.28	0.84
(2,2652)	1:95:A:LEU:HD21	1:107:A:ASP:HB2	12	0.78	0.28	0.84
(2,3271)	1:28:A:LEU:HD11	1:25:A:LYS:HD2	12	0.55	0.39	0.48
(2,3271)	1:28:A:LEU:HD13	1:25:A:LYS:HD3	12	0.55	0.39	0.48
(2,3271)	1:28:A:LEU:HD11	1:25:A:LYS:HD3	12	0.55	0.39	0.48
(2,3271)	1:28:A:LEU:HD12	1:25:A:LYS:HD3	12	0.55	0.39	0.48
(2,3271)	1:28:A:LEU:HD13	1:25:A:LYS:HD2	12	0.55	0.39	0.48
(2,3271)	1:58:A:LEU:HD22	1:25:A:LYS:HD3	12	0.55	0.39	0.48
(2,3271)	1:58:A:LEU:HD23	1:25:A:LYS:HD2	12	0.55	0.39	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3271)	1:58:A:LEU:HD22	1:25:A:LYS:HD2	12	0.55	0.39	0.48
(2,3271)	1:58:A:LEU:HD21	1:25:A:LYS:HD2	12	0.55	0.39	0.48
(2,4276)	1:111:A:LEU:HD21	1:114:A:GLU:HB2	12	0.41	0.09	0.43
(2,4276)	1:111:A:LEU:HD23	1:114:A:GLU:HB2	12	0.41	0.09	0.43
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	12	0.38	0.18	0.35
(2,527)	1:72:A:LYS:HB2	1:79:A:TYR:H	12	0.32	0.11	0.3
(2,527)	1:72:A:LYS:HD3	1:79:A:TYR:H	12	0.32	0.11	0.3
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG22	12	0.24	0.07	0.26
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG23	12	0.24	0.07	0.26
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG21	12	0.24	0.07	0.26
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	12	0.2	0.05	0.22
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	12	0.19	0.08	0.16
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	12	0.19	0.02	0.19
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	12	0.18	0.04	0.18
(2,1731)	1:56:A:ILE:HG22	1:24:A:ILE:HA	12	0.16	0.04	0.15
(2,1731)	1:56:A:ILE:HG21	1:24:A:ILE:HA	12	0.16	0.04	0.15
(2,1731)	1:56:A:ILE:HG23	1:24:A:ILE:HA	12	0.16	0.04	0.15
(2,316)	1:26:A:ASP:HB3	1:32:A:LEU:H	11	0.79	0.15	0.8
(2,316)	1:31:A:LYS:HE2	1:32:A:LEU:H	11	0.79	0.15	0.8
(2,316)	1:31:A:LYS:HE3	1:32:A:LEU:H	11	0.79	0.15	0.8
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	11	0.66	0.15	0.72
(2,3409)	1:79:A:TYR:HD1	1:123:A:LEU:HD21	11	0.62	0.21	0.68
(2,3409)	1:59:A:TYR:HE2	1:60:A:LEU:HD21	11	0.62	0.21	0.68
(2,3409)	1:59:A:TYR:HE1	1:60:A:LEU:HD21	11	0.62	0.21	0.68
(2,3409)	1:79:A:TYR:HD2	1:123:A:LEU:HD21	11	0.62	0.21	0.68
(2,1389)	1:106:A:VAL:HG11	1:105:A:ASN:HD21	11	0.61	0.3	0.76
(2,1389)	1:106:A:VAL:HG12	1:105:A:ASN:HD21	11	0.61	0.3	0.76
(2,1389)	1:106:A:VAL:HG23	1:105:A:ASN:HD21	11	0.61	0.3	0.76
(2,1389)	1:106:A:VAL:HG13	1:105:A:ASN:HD21	11	0.61	0.3	0.76
(2,1389)	1:106:A:VAL:HG21	1:105:A:ASN:HD21	11	0.61	0.3	0.76
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE1	11	0.54	0.21	0.64
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE2	11	0.54	0.21	0.64
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE1	11	0.54	0.21	0.64
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE2	11	0.54	0.21	0.64
(2,1899)	1:76:A:ILE:HD11	1:73:A:SER:HB2	11	0.51	0.24	0.47
(2,1899)	1:76:A:ILE:HD12	1:73:A:SER:HB3	11	0.51	0.24	0.47
(2,1899)	1:76:A:ILE:HD13	1:73:A:SER:HB3	11	0.51	0.24	0.47
(2,1899)	1:76:A:ILE:HG23	1:73:A:SER:HB3	11	0.51	0.24	0.47
(2,1899)	1:76:A:ILE:HG23	1:73:A:SER:HB2	11	0.51	0.24	0.47
(2,1899)	1:76:A:ILE:HD11	1:73:A:SER:HB3	11	0.51	0.24	0.47
(2,1899)	1:76:A:ILE:HG22	1:73:A:SER:HB2	11	0.51	0.24	0.47
(2,510)	1:65:A:LYS:HE3	1:64:A:VAL:H	11	0.48	0.17	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,510)	1:65:A:LYS:HE2	1:64:A:VAL:H	11	0.48	0.17	0.51
(2,510)	1:59:A:TYR:HB2	1:64:A:VAL:H	11	0.48	0.17	0.51
(2,4377)	1:112:A:LEU:HD13	1:109:A:GLU:HG3	11	0.35	0.15	0.31
(2,4377)	1:135:A:LEU:HD22	1:134:A:GLU:HG3	11	0.35	0.15	0.31
(2,4377)	1:112:A:LEU:HD12	1:109:A:GLU:HG3	11	0.35	0.15	0.31
(2,4377)	1:135:A:LEU:HD21	1:134:A:GLU:HG3	11	0.35	0.15	0.31
(2,4377)	1:112:A:LEU:HD11	1:109:A:GLU:HG3	11	0.35	0.15	0.31
(2,4377)	1:135:A:LEU:HD23	1:134:A:GLU:HG3	11	0.35	0.15	0.31
(2,4667)	1:94:A:LEU:HD22	1:115:A:TYR:HE1	11	0.3	0.11	0.29
(2,4667)	1:94:A:LEU:HD22	1:115:A:TYR:HE2	11	0.3	0.11	0.29
(2,4667)	1:94:A:LEU:HD21	1:115:A:TYR:HE1	11	0.3	0.11	0.29
(2,4667)	1:94:A:LEU:HD23	1:115:A:TYR:HE2	11	0.3	0.11	0.29
(2,4667)	1:111:A:LEU:HD23	1:115:A:TYR:HE2	11	0.3	0.11	0.29
(2,4667)	1:111:A:LEU:HD21	1:115:A:TYR:HE1	11	0.3	0.11	0.29
(2,4667)	1:123:A:LEU:HD21	1:79:A:TYR:HE2	11	0.3	0.11	0.29
(2,1200)	1:43:A:GLU:HG3	1:41:A:TYR:H	11	0.24	0.08	0.25
(2,1200)	1:36:A:LEU:HB3	1:41:A:TYR:H	11	0.24	0.08	0.25
(2,1540)	1:46:A:LYS:HB2	1:30:A:GLY:H	11	0.23	0.06	0.22
(2,1540)	1:31:A:LYS:HB3	1:30:A:GLY:H	11	0.23	0.06	0.22
(2,2099)	1:131:A:GLU:HG2	1:131:A:GLU:HA	11	0.22	0.05	0.21
(2,2099)	1:134:A:GLU:HG2	1:134:A:GLU:HA	11	0.22	0.05	0.21
(2,2099)	1:134:A:GLU:HG2	1:131:A:GLU:HA	11	0.22	0.05	0.21
(2,4398)	1:52:A:LEU:HA	1:55:A:ARG:HD2	11	0.2	0.07	0.19
(2,4398)	1:52:A:LEU:HA	1:55:A:ARG:HD3	11	0.2	0.07	0.19
(2,4398)	1:113:A:ARG:HA	1:113:A:ARG:HD2	11	0.2	0.07	0.19
(2,4398)	1:113:A:ARG:HA	1:113:A:ARG:HD3	11	0.2	0.07	0.19
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	11	0.2	0.07	0.2
(2,3911)	1:70:A:PHE:HE1	1:103:A:ILE:HG21	11	0.18	0.05	0.18
(2,3911)	1:70:A:PHE:HE2	1:103:A:ILE:HG23	11	0.18	0.05	0.18
(2,3911)	1:70:A:PHE:HE1	1:103:A:ILE:HG22	11	0.18	0.05	0.18
(2,3911)	1:70:A:PHE:HE2	1:103:A:ILE:HG21	11	0.18	0.05	0.18
(2,3911)	1:70:A:PHE:HE2	1:103:A:ILE:HG22	11	0.18	0.05	0.18
(2,3911)	1:70:A:PHE:HE1	1:103:A:ILE:HG23	11	0.18	0.05	0.18
(2,2318)	1:50:A:GLU:HB2	1:47:A:ASP:HA	11	0.17	0.08	0.13
(2,2318)	1:110:A:LYS:HB2	1:107:A:ASP:HA	11	0.17	0.08	0.13
(2,3265)	1:94:A:LEU:HD11	1:91:A:ILE:HG12	11	0.16	0.03	0.16
(2,3265)	1:94:A:LEU:HD13	1:91:A:ILE:HG12	11	0.16	0.03	0.16
(2,3265)	1:94:A:LEU:HD12	1:91:A:ILE:HG12	11	0.16	0.03	0.16
(2,3111)	1:22:A:VAL:HA	1:65:A:LYS:HD3	10	0.65	0.25	0.55
(2,3111)	1:21:A:TYR:HA	1:65:A:LYS:HD3	10	0.65	0.25	0.55
(2,3111)	1:79:A:TYR:HA	1:72:A:LYS:HD3	10	0.65	0.25	0.55
(2,4092)	1:14:A:PHE:HD1	1:122:A:ILE:HD12	10	0.56	0.28	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4092)	1:14:A:PHE:HD2	1:122:A:ILE:HD12	10	0.56	0.28	0.56
(2,4092)	1:14:A:PHE:HD2	1:122:A:ILE:HD13	10	0.56	0.28	0.56
(2,4092)	1:14:A:PHE:HD2	1:122:A:ILE:HD11	10	0.56	0.28	0.56
(2,4092)	1:14:A:PHE:HD1	1:122:A:ILE:HD11	10	0.56	0.28	0.56
(2,1036)	1:43:A:GLU:HG2	1:33:A:LYS:H	10	0.44	0.16	0.4
(2,1036)	1:34:A:ILE:HB	1:33:A:LYS:H	10	0.44	0.16	0.4
(2,2074)	1:25:A:LYS:HE3	1:25:A:LYS:HA	10	0.39	0.11	0.42
(2,2074)	1:61:A:TRP:HB2	1:25:A:LYS:HA	10	0.39	0.11	0.42
(2,2074)	1:25:A:LYS:HE2	1:25:A:LYS:HA	10	0.39	0.11	0.42
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG21	10	0.35	0.19	0.33
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG23	10	0.35	0.19	0.33
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG22	10	0.35	0.19	0.33
(2,3925)	1:21:A:TYR:HE1	1:34:A:ILE:HG21	10	0.35	0.19	0.33
(2,3201)	1:51:A:LYS:HE3	1:114:A:GLU:HB2	10	0.32	0.11	0.34
(2,3201)	1:115:A:TYR:HB2	1:114:A:GLU:HB2	10	0.32	0.11	0.34
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD11	10	0.32	0.17	0.25
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD13	10	0.32	0.17	0.25
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD12	10	0.32	0.17	0.25
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD13	10	0.32	0.14	0.32
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD12	10	0.32	0.14	0.32
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD11	10	0.32	0.14	0.32
(2,2653)	1:95:A:LEU:HD12	1:107:A:ASP:HB2	10	0.31	0.08	0.32
(2,2653)	1:95:A:LEU:HD11	1:107:A:ASP:HB2	10	0.31	0.08	0.32
(2,2653)	1:95:A:LEU:HD13	1:107:A:ASP:HB2	10	0.31	0.08	0.32
(2,4385)	1:129:A:TYR:HB3	1:131:A:GLU:HG3	10	0.28	0.13	0.26
(2,4385)	1:46:A:LYS:HE2	1:50:A:GLU:HG2	10	0.28	0.13	0.26
(2,156)	1:69:A:ILE:HD11	1:120:A:PHE:H	10	0.27	0.14	0.23
(2,156)	1:69:A:ILE:HD12	1:120:A:PHE:H	10	0.27	0.14	0.23
(2,156)	1:69:A:ILE:HD13	1:120:A:PHE:H	10	0.27	0.14	0.23
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG12	10	0.26	0.16	0.16
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG11	10	0.26	0.16	0.16
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG13	10	0.26	0.16	0.16
(2,3085)	1:21:A:TYR:HD1	1:20:A:GLU:HB2	10	0.24	0.08	0.22
(2,3085)	1:21:A:TYR:HD2	1:20:A:GLU:HB2	10	0.24	0.08	0.22
(2,816)	1:51:A:LYS:HG2	1:49:A:VAL:H	10	0.21	0.1	0.16
(2,816)	1:52:A:LEU:HB2	1:49:A:VAL:H	10	0.21	0.1	0.16
(2,816)	1:51:A:LYS:HG3	1:49:A:VAL:H	10	0.21	0.1	0.16
(2,1350)	1:50:A:GLU:HB3	1:53:A:SER:H	10	0.21	0.07	0.2
(2,1350)	1:51:A:LYS:HB2	1:53:A:SER:H	10	0.21	0.07	0.2
(2,158)	1:122:A:ILE:HG22	1:123:A:LEU:H	10	0.2	0.05	0.22
(2,158)	1:123:A:LEU:HD23	1:123:A:LEU:H	10	0.2	0.05	0.22
(2,158)	1:122:A:ILE:HG21	1:123:A:LEU:H	10	0.2	0.05	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,158)	1:122:A:ILE:HG23	1:123:A:LEU:H	10	0.2	0.05	0.22
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB2	10	0.2	0.04	0.22
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB3	10	0.2	0.04	0.22
(2,2806)	1:15:A:SER:HB2	1:38:A:ASN:HB2	10	0.2	0.04	0.22
(2,2806)	1:15:A:SER:HB3	1:38:A:ASN:HB2	10	0.2	0.04	0.22
(2,764)	1:29:A:ASP:HB3	1:28:A:LEU:H	10	0.2	0.06	0.18
(2,764)	1:46:A:LYS:HE2	1:28:A:LEU:H	10	0.2	0.06	0.18
(2,2960)	1:52:A:LEU:HA	1:114:A:GLU:HG3	10	0.19	0.06	0.18
(2,819)	1:112:A:LEU:HB2	1:111:A:LEU:H	10	0.19	0.05	0.18
(2,819)	1:110:A:LYS:HD3	1:111:A:LEU:H	10	0.19	0.05	0.18
(2,819)	1:110:A:LYS:HD2	1:111:A:LEU:H	10	0.19	0.05	0.18
(2,1948)	1:92:A:SER:H	1:99:A:ILE:HA	10	0.19	0.08	0.17
(2,1654)	1:41:A:TYR:HB3	1:36:A:LEU:H	10	0.16	0.04	0.16
(2,1030)	1:22:A:VAL:HB	1:29:A:ASP:H	10	0.16	0.06	0.15
(2,1833)	1:51:A:LYS:HB2	1:54:A:SER:HB2	9	0.57	0.31	0.54
(2,1833)	1:50:A:GLU:HB3	1:54:A:SER:HB2	9	0.57	0.31	0.54
(2,1833)	1:132:A:GLU:HB2	1:133:A:THR:HA	9	0.57	0.31	0.54
(2,3050)	1:142:A:HIS:HD2	1:142:A:HIS:HB3	9	0.32	0.1	0.36
(2,3050)	1:143:A:HIS:HD2	1:143:A:HIS:HB3	9	0.32	0.1	0.36
(2,4459)	1:33:A:LYS:HB3	1:41:A:TYR:HD1	9	0.27	0.1	0.3
(2,4459)	1:33:A:LYS:HB3	1:41:A:TYR:HD2	9	0.27	0.1	0.3
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG23	9	0.26	0.1	0.23
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG22	9	0.26	0.1	0.23
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG21	9	0.26	0.1	0.23
(2,4648)	1:20:A:GLU:HA	1:21:A:TYR:HE1	9	0.25	0.09	0.32
(2,4648)	1:20:A:GLU:HA	1:21:A:TYR:HE2	9	0.25	0.09	0.32
(2,225)	1:98:A:GLU:HG2	1:99:A:ILE:H	9	0.25	0.15	0.21
(2,225)	1:98:A:GLU:HG3	1:99:A:ILE:H	9	0.25	0.15	0.21
(2,962)	1:95:A:LEU:HA	1:97:A:ARG:H	9	0.24	0.1	0.2
(2,1386)	1:65:A:LYS:HD3	1:21:A:TYR:H	9	0.24	0.08	0.21
(2,1386)	1:65:A:LYS:HD2	1:21:A:TYR:H	9	0.24	0.08	0.21
(2,2954)	1:137:A:GLU:HA	1:137:A:GLU:HG2	9	0.2	0.05	0.2
(2,2954)	1:132:A:GLU:HA	1:132:A:GLU:HG2	9	0.2	0.05	0.2
(2,4320)	1:24:A:ILE:HB	1:66:A:ILE:HG23	9	0.18	0.06	0.21
(2,4320)	1:24:A:ILE:HB	1:66:A:ILE:HG22	9	0.18	0.06	0.21
(2,2340)	1:114:A:GLU:HB3	1:115:A:TYR:HA	9	0.16	0.04	0.17
(2,1523)	1:63:A:LEU:HG	1:62:A:SER:H	9	0.12	0.01	0.12
(2,3353)	1:24:A:ILE:H	1:25:A:LYS:HG2	8	0.87	0.06	0.86
(2,3353)	1:24:A:ILE:H	1:25:A:LYS:HG3	8	0.87	0.06	0.86
(2,2651)	1:95:A:LEU:HD22	1:110:A:LYS:HE3	8	0.67	0.19	0.67
(2,2651)	1:95:A:LEU:HD23	1:110:A:LYS:HE3	8	0.67	0.19	0.67
(2,2651)	1:22:A:VAL:HG12	1:31:A:LYS:HE3	8	0.67	0.19	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2651)	1:22:A:VAL:HG11	1:31:A:LYS:HE3	8	0.67	0.19	0.67
(2,2651)	1:95:A:LEU:HD21	1:110:A:LYS:HE3	8	0.67	0.19	0.67
(2,3299)	1:44:A:ILE:H	1:33:A:LYS:HG2	8	0.43	0.13	0.39
(2,4469)	1:69:A:ILE:HD12	1:21:A:TYR:HD2	8	0.36	0.16	0.35
(2,4469)	1:35:A:ARG:HG3	1:41:A:TYR:HD2	8	0.36	0.16	0.35
(2,4469)	1:69:A:ILE:HD13	1:21:A:TYR:HD1	8	0.36	0.16	0.35
(2,4469)	1:69:A:ILE:HD13	1:21:A:TYR:HD2	8	0.36	0.16	0.35
(2,4505)	1:122:A:ILE:HD12	1:14:A:PHE:HD1	8	0.36	0.15	0.37
(2,4505)	1:122:A:ILE:HD12	1:14:A:PHE:HD2	8	0.36	0.15	0.37
(2,4505)	1:122:A:ILE:HD13	1:14:A:PHE:HD2	8	0.36	0.15	0.37
(2,4505)	1:122:A:ILE:HG23	1:14:A:PHE:HD2	8	0.36	0.15	0.37
(2,4505)	1:122:A:ILE:HG22	1:14:A:PHE:HD1	8	0.36	0.15	0.37
(2,4505)	1:122:A:ILE:HG22	1:14:A:PHE:HD2	8	0.36	0.15	0.37
(2,4505)	1:122:A:ILE:HD11	1:14:A:PHE:HD2	8	0.36	0.15	0.37
(2,1847)	1:75:A:GLU:HB2	1:73:A:SER:HB3	8	0.34	0.15	0.36
(2,1847)	1:78:A:GLU:HB3	1:73:A:SER:HB2	8	0.34	0.15	0.36
(2,3017)	1:66:A:ILE:H	1:65:A:LYS:HD3	8	0.32	0.08	0.29
(2,3017)	1:104:A:LEU:H	1:97:A:ARG:HG3	8	0.32	0.08	0.29
(2,1435)	1:31:A:LYS:HB3	1:23:A:THR:H	8	0.32	0.09	0.31
(2,1435)	1:25:A:LYS:HB3	1:23:A:THR:H	8	0.32	0.09	0.31
(2,784)	1:61:A:TRP:HB2	1:24:A:ILE:H	8	0.21	0.06	0.22
(2,29)	1:48:A:GLU:HG3	1:46:A:LYS:H	8	0.18	0.08	0.15
(2,3281)	1:72:A:LYS:H	1:71:A:ILE:HG13	8	0.16	0.03	0.16
(2,2634)	1:35:A:ARG:HB3	1:35:A:ARG:HD3	8	0.16	0.02	0.16
(2,2634)	1:35:A:ARG:HB2	1:35:A:ARG:HD3	8	0.16	0.02	0.16
(2,1188)	1:37:A:ASN:HB2	1:15:A:SER:H	8	0.15	0.04	0.15
(2,1188)	1:37:A:ASN:HB3	1:15:A:SER:H	8	0.15	0.04	0.15
(2,886)	1:28:A:LEU:HD11	1:26:A:ASP:H	8	0.15	0.05	0.14
(2,886)	1:24:A:ILE:HG22	1:26:A:ASP:H	8	0.15	0.05	0.14
(2,886)	1:28:A:LEU:HD12	1:26:A:ASP:H	8	0.15	0.05	0.14
(2,886)	1:24:A:ILE:HG23	1:26:A:ASP:H	8	0.15	0.05	0.14
(2,568)	1:49:A:VAL:HG11	1:50:A:GLU:H	8	0.14	0.03	0.13
(2,568)	1:49:A:VAL:HG12	1:50:A:GLU:H	8	0.14	0.03	0.13
(2,568)	1:49:A:VAL:HG13	1:50:A:GLU:H	8	0.14	0.03	0.13
(2,844)	1:94:A:LEU:HD21	1:94:A:LEU:H	8	0.13	0.02	0.14
(2,844)	1:94:A:LEU:HD23	1:94:A:LEU:H	8	0.13	0.02	0.14
(2,3681)	1:74:A:SER:H	1:126:A:THR:HG23	7	0.7	0.31	0.8
(2,3681)	1:129:A:TYR:H	1:126:A:THR:HG23	7	0.7	0.31	0.8
(2,3681)	1:75:A:GLU:H	1:126:A:THR:HG22	7	0.7	0.31	0.8
(2,3681)	1:75:A:GLU:H	1:126:A:THR:HG21	7	0.7	0.31	0.8
(2,1677)	1:65:A:LYS:HE2	1:23:A:THR:HB	7	0.5	0.2	0.46
(2,1677)	1:65:A:LYS:HE3	1:23:A:THR:HB	7	0.5	0.2	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3435)	1:23:A:THR:HB	1:65:A:LYS:HG3	7	0.33	0.12	0.34
(2,3435)	1:22:A:VAL:HA	1:65:A:LYS:HG3	7	0.33	0.12	0.34
(2,3405)	1:115:A:TYR:HE2	1:118:A:LEU:HD11	7	0.21	0.07	0.2
(2,3405)	1:115:A:TYR:HE2	1:118:A:LEU:HD13	7	0.21	0.07	0.2
(2,3405)	1:115:A:TYR:HE1	1:118:A:LEU:HD12	7	0.21	0.07	0.2
(2,3405)	1:115:A:TYR:HE1	1:118:A:LEU:HD13	7	0.21	0.07	0.2
(2,3405)	1:68:A:PHE:HZ	1:118:A:LEU:HD13	7	0.21	0.07	0.2
(2,3405)	1:115:A:TYR:HE2	1:118:A:LEU:HD12	7	0.21	0.07	0.2
(2,677)	1:78:A:GLU:HA	1:103:A:ILE:H	7	0.17	0.05	0.17
(2,791)	1:111:A:LEU:HB3	1:112:A:LEU:H	7	0.17	0.04	0.16
(2,4012)	1:68:A:PHE:HB3	1:66:A:ILE:HG22	7	0.16	0.04	0.15
(2,4012)	1:68:A:PHE:HB3	1:66:A:ILE:HG21	7	0.16	0.04	0.15
(2,4012)	1:68:A:PHE:HB3	1:66:A:ILE:HG23	7	0.16	0.04	0.15
(2,1599)	1:62:A:SER:HA	1:26:A:ASP:H	7	0.16	0.05	0.15
(2,1599)	1:141:A:HIS:HA	1:140:A:GLU:H	7	0.16	0.05	0.15
(2,123)	1:28:A:LEU:HA	1:31:A:LYS:H	7	0.14	0.02	0.15
(2,980)	1:141:A:HIS:HB2	1:141:A:HIS:H	7	0.14	0.04	0.14
(2,1399)	1:93:A:ILE:HG23	1:55:A:ARG:HE	6	1.1	0.17	1.14
(2,1399)	1:56:A:ILE:HG22	1:55:A:ARG:HE	6	1.1	0.17	1.14
(2,1399)	1:56:A:ILE:HG21	1:55:A:ARG:HE	6	1.1	0.17	1.14
(2,1399)	1:56:A:ILE:HG23	1:55:A:ARG:HE	6	1.1	0.17	1.14
(2,1399)	1:93:A:ILE:HG21	1:55:A:ARG:HE	6	1.1	0.17	1.14
(2,3609)	1:126:A:THR:HG23	1:125:A:PRO:HG2	6	0.78	0.43	0.64
(2,3609)	1:13:A:ILE:HG13	1:125:A:PRO:HG2	6	0.78	0.43	0.64
(2,3705)	1:14:A:PHE:HD1	1:10:A:LEU:HD23	6	0.56	0.21	0.52
(2,3705)	1:14:A:PHE:HD2	1:10:A:LEU:HD23	6	0.56	0.21	0.52
(2,3705)	1:14:A:PHE:HD2	1:10:A:LEU:HD22	6	0.56	0.21	0.52
(2,118)	1:125:A:PRO:HD3	1:123:A:LEU:H	6	0.49	0.34	0.42
(2,118)	1:124:A:SER:HB3	1:123:A:LEU:H	6	0.49	0.34	0.42
(2,118)	1:124:A:SER:HB2	1:123:A:LEU:H	6	0.49	0.34	0.42
(2,4374)	1:135:A:LEU:HD22	1:134:A:GLU:HB3	6	0.42	0.08	0.43
(2,4374)	1:135:A:LEU:HD21	1:134:A:GLU:HB3	6	0.42	0.08	0.43
(2,4374)	1:135:A:LEU:HD11	1:131:A:GLU:HB2	6	0.42	0.08	0.43
(2,4374)	1:135:A:LEU:HD13	1:131:A:GLU:HB2	6	0.42	0.08	0.43
(2,1990)	1:14:A:PHE:HD2	1:11:A:LYS:HA	6	0.3	0.13	0.33
(2,1990)	1:68:A:PHE:HD2	1:66:A:ILE:HA	6	0.3	0.13	0.33
(2,1990)	1:14:A:PHE:HD1	1:11:A:LYS:HA	6	0.3	0.13	0.33
(2,1990)	1:68:A:PHE:HD1	1:66:A:ILE:HA	6	0.3	0.13	0.33
(2,1222)	1:33:A:LYS:HD2	1:41:A:TYR:H	6	0.29	0.2	0.2
(2,1222)	1:33:A:LYS:HD3	1:41:A:TYR:H	6	0.29	0.2	0.2
(2,3601)	1:56:A:ILE:HB	1:52:A:LEU:HD11	6	0.29	0.14	0.24
(2,3601)	1:118:A:LEU:HB3	1:52:A:LEU:HD22	6	0.29	0.14	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3601)	1:56:A:ILE:HB	1:52:A:LEU:HD12	6	0.29	0.14	0.24
(2,3601)	1:56:A:ILE:HB	1:52:A:LEU:HD13	6	0.29	0.14	0.24
(2,4641)	1:78:A:GLU:HA	1:79:A:TYR:HE2	6	0.26	0.12	0.26
(2,4641)	1:115:A:TYR:HA	1:115:A:TYR:HE2	6	0.26	0.12	0.26
(2,4641)	1:78:A:GLU:HA	1:79:A:TYR:HE1	6	0.26	0.12	0.26
(2,2494)	1:10:A:LEU:HG	1:9:A:GLY:HA2	6	0.26	0.07	0.27
(2,2494)	1:10:A:LEU:HB2	1:9:A:GLY:HA2	6	0.26	0.07	0.27
(2,1445)	1:65:A:LYS:HG2	1:23:A:THR:H	6	0.25	0.08	0.22
(2,3826)	1:79:A:TYR:HB2	1:108:A:VAL:HG13	6	0.24	0.06	0.26
(2,3826)	1:79:A:TYR:HB2	1:108:A:VAL:HG11	6	0.24	0.06	0.26
(2,3826)	1:79:A:TYR:HB2	1:108:A:VAL:HG12	6	0.24	0.06	0.26
(2,3826)	1:109:A:GLU:HG3	1:108:A:VAL:HG12	6	0.24	0.06	0.26
(2,1330)	1:137:A:GLU:HG2	1:136:A:SER:H	6	0.22	0.16	0.16
(2,1330)	1:132:A:GLU:HG2	1:136:A:SER:H	6	0.22	0.16	0.16
(2,1191)	1:131:A:GLU:HG2	1:133:A:THR:H	6	0.21	0.08	0.19
(2,1191)	1:132:A:GLU:HG2	1:133:A:THR:H	6	0.21	0.08	0.19
(2,2825)	1:25:A:LYS:HB3	1:26:A:ASP:HB2	6	0.2	0.07	0.18
(2,2825)	1:31:A:LYS:HB3	1:26:A:ASP:HB2	6	0.2	0.07	0.18
(2,1718)	1:64:A:VAL:HB	1:24:A:ILE:HA	6	0.18	0.04	0.18
(2,2235)	1:95:A:LEU:H	1:90:A:ALA:HA	6	0.16	0.02	0.16
(2,3908)	1:48:A:GLU:H	1:44:A:ILE:HG21	6	0.14	0.03	0.14
(2,3908)	1:48:A:GLU:H	1:44:A:ILE:HG22	6	0.14	0.03	0.14
(2,2356)	1:19:A:ALA:HB1	1:36:A:LEU:HA	6	0.13	0.02	0.12
(2,2356)	1:19:A:ALA:HB3	1:36:A:LEU:HA	6	0.13	0.02	0.12
(2,2356)	1:19:A:ALA:HB2	1:36:A:LEU:HA	6	0.13	0.02	0.12
(2,1229)	1:130:A:THR:HG21	1:130:A:THR:H	6	0.11	0.01	0.11
(2,1229)	1:130:A:THR:HG22	1:130:A:THR:H	6	0.11	0.01	0.11
(2,1229)	1:130:A:THR:HG23	1:130:A:THR:H	6	0.11	0.01	0.11
(2,3280)	1:79:A:TYR:H	1:104:A:LEU:HG	5	0.65	0.07	0.68
(2,1314)	1:100:A:SER:HB2	1:101:A:ASN:HD21	5	0.47	0.15	0.54
(2,1314)	1:100:A:SER:HB3	1:101:A:ASN:HD21	5	0.47	0.15	0.54
(2,1220)	1:99:A:ILE:HG13	1:101:A:ASN:H	5	0.28	0.1	0.27
(2,1017)	1:45:A:LYS:HD3	1:117:A:SER:H	5	0.27	0.13	0.35
(2,1017)	1:45:A:LYS:HD2	1:117:A:SER:H	5	0.27	0.13	0.35
(2,1440)	1:20:A:GLU:HG2	1:35:A:ARG:HE	5	0.23	0.08	0.25
(2,3803)	1:42:A:HIS:HB2	1:36:A:LEU:HD22	5	0.22	0.08	0.27
(2,3803)	1:42:A:HIS:HB2	1:36:A:LEU:HD21	5	0.22	0.08	0.27
(2,3803)	1:42:A:HIS:HB2	1:36:A:LEU:HD23	5	0.22	0.08	0.27
(2,108)	1:67:A:PRO:HA	1:120:A:PHE:H	5	0.22	0.06	0.22
(2,2819)	1:81:A:VAL:HB	1:101:A:ASN:HB2	5	0.22	0.1	0.18
(2,4011)	1:68:A:PHE:HB3	1:119:A:ILE:HG21	5	0.21	0.1	0.15
(2,4011)	1:68:A:PHE:HB3	1:119:A:ILE:HG23	5	0.21	0.1	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4011)	1:68:A:PHE:HB3	1:119:A:ILE:HG22	5	0.21	0.1	0.15
(2,4644)	1:123:A:LEU:HA	1:79:A:TYR:HE1	5	0.2	0.06	0.21
(2,4644)	1:123:A:LEU:HA	1:79:A:TYR:HE2	5	0.2	0.06	0.21
(2,1199)	1:102:A:VAL:HB	1:101:A:ASN:H	5	0.2	0.05	0.21
(2,1199)	1:99:A:ILE:HB	1:101:A:ASN:H	5	0.2	0.05	0.21
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG11	5	0.18	0.05	0.17
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG12	5	0.18	0.05	0.17
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG13	5	0.18	0.05	0.17
(2,582)	1:56:A:ILE:HG13	1:55:A:ARG:H	5	0.17	0.04	0.19
(2,4279)	1:68:A:PHE:HD2	1:118:A:LEU:HD12	5	0.17	0.07	0.13
(2,4279)	1:68:A:PHE:HD1	1:118:A:LEU:HD12	5	0.17	0.07	0.13
(2,4279)	1:68:A:PHE:HD2	1:118:A:LEU:HD11	5	0.17	0.07	0.13
(2,4279)	1:68:A:PHE:HD1	1:118:A:LEU:HD11	5	0.17	0.07	0.13
(2,3714)	1:49:A:VAL:H	1:28:A:LEU:HD21	5	0.17	0.07	0.13
(2,3714)	1:49:A:VAL:H	1:28:A:LEU:HD23	5	0.17	0.07	0.13
(2,1804)	1:100:A:SER:HA	1:100:A:SER:HB2	5	0.16	0.0	0.16
(2,1496)	1:71:A:ILE:HG12	1:83:A:GLY:H	5	0.16	0.01	0.16
(2,2298)	1:3:A:ASP:HB3	1:3:A:ASP:HA	5	0.15	0.01	0.15
(2,4291)	1:52:A:LEU:HG	1:94:A:LEU:HD11	5	0.15	0.02	0.15
(2,4291)	1:52:A:LEU:HG	1:94:A:LEU:HD13	5	0.15	0.02	0.15
(2,1244)	1:34:A:ILE:HD11	1:20:A:GLU:H	5	0.15	0.03	0.16
(2,1244)	1:34:A:ILE:HD13	1:20:A:GLU:H	5	0.15	0.03	0.16
(2,2466)	1:69:A:ILE:HG22	1:70:A:PHE:HA	5	0.14	0.02	0.15
(2,2466)	1:69:A:ILE:HG23	1:70:A:PHE:HA	5	0.14	0.02	0.15
(2,4324)	1:91:A:ILE:H	1:56:A:ILE:HD13	5	0.13	0.02	0.12
(2,4324)	1:91:A:ILE:H	1:56:A:ILE:HD11	5	0.13	0.02	0.12
(2,3614)	1:60:A:LEU:HB2	1:64:A:VAL:HG21	5	0.12	0.01	0.12
(2,3614)	1:60:A:LEU:HB2	1:64:A:VAL:HG22	5	0.12	0.01	0.12
(2,293)	1:129:A:TYR:HA	1:129:A:TYR:H	5	0.12	0.01	0.11
(2,700)	1:140:A:GLU:HA	1:140:A:GLU:H	5	0.1	0.0	0.1
(2,3794)	1:124:A:SER:HB3	1:126:A:THR:HG22	4	1.11	0.38	1.27
(2,3794)	1:124:A:SER:HB2	1:126:A:THR:HG23	4	1.11	0.38	1.27
(2,3794)	1:124:A:SER:HB3	1:126:A:THR:HG23	4	1.11	0.38	1.27
(2,2842)	1:25:A:LYS:HB2	1:26:A:ASP:HB2	4	0.54	0.13	0.59
(2,1378)	1:109:A:GLU:HB2	1:105:A:ASN:HD22	4	0.41	0.17	0.48
(2,1378)	1:106:A:VAL:HB	1:105:A:ASN:HD22	4	0.41	0.17	0.48
(2,1680)	1:125:A:PRO:HB2	1:126:A:THR:HB	4	0.38	0.08	0.36
(2,1394)	1:64:A:VAL:HG22	1:87:A:ASN:HD22	4	0.32	0.16	0.25
(2,1394)	1:64:A:VAL:HG23	1:87:A:ASN:HD22	4	0.32	0.16	0.25
(2,2841)	1:106:A:VAL:HG12	1:105:A:ASN:HB3	4	0.31	0.08	0.34
(2,2841)	1:72:A:LYS:HG2	1:105:A:ASN:HB3	4	0.31	0.08	0.34
(2,2841)	1:106:A:VAL:HG11	1:105:A:ASN:HB3	4	0.31	0.08	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2841)	1:106:A:VAL:HG13	1:105:A:ASN:HB2	4	0.31	0.08	0.34
(2,1542)	1:31:A:LYS:HG2	1:30:A:GLY:H	4	0.28	0.06	0.29
(2,1542)	1:46:A:LYS:HG3	1:30:A:GLY:H	4	0.28	0.06	0.29
(2,1542)	1:28:A:LEU:HB2	1:30:A:GLY:H	4	0.28	0.06	0.29
(2,1601)	1:20:A:GLU:HG3	1:34:A:ILE:H	4	0.28	0.14	0.24
(2,1601)	1:43:A:GLU:HG3	1:34:A:ILE:H	4	0.28	0.14	0.24
(2,4116)	1:115:A:TYR:HA	1:119:A:ILE:HD13	4	0.24	0.07	0.22
(2,4116)	1:115:A:TYR:HA	1:119:A:ILE:HD11	4	0.24	0.07	0.22
(2,4116)	1:115:A:TYR:HA	1:119:A:ILE:HD12	4	0.24	0.07	0.22
(2,100)	1:79:A:TYR:HE1	1:70:A:PHE:H	4	0.23	0.16	0.15
(2,100)	1:79:A:TYR:HE2	1:70:A:PHE:H	4	0.23	0.16	0.15
(2,161)	1:69:A:ILE:HG21	1:70:A:PHE:H	4	0.22	0.06	0.24
(2,161)	1:69:A:ILE:HG22	1:70:A:PHE:H	4	0.22	0.06	0.24
(2,1787)	1:120:A:PHE:HE2	1:17:A:SER:HB3	4	0.22	0.13	0.17
(2,1787)	1:21:A:TYR:HE1	1:17:A:SER:HB3	4	0.22	0.13	0.17
(2,2845)	1:51:A:LYS:HG2	1:47:A:ASP:HB2	4	0.21	0.08	0.2
(2,2845)	1:51:A:LYS:HG3	1:47:A:ASP:HB2	4	0.21	0.08	0.2
(2,2955)	1:75:A:GLU:HA	1:75:A:GLU:HG2	4	0.2	0.05	0.22
(2,2955)	1:75:A:GLU:HA	1:75:A:GLU:HG3	4	0.2	0.05	0.22
(2,544)	1:10:A:LEU:HG	1:10:A:LEU:H	4	0.19	0.03	0.2
(2,401)	1:70:A:PHE:HE1	1:69:A:ILE:H	4	0.18	0.05	0.2
(2,401)	1:70:A:PHE:HE2	1:69:A:ILE:H	4	0.18	0.05	0.2
(2,2372)	1:34:A:ILE:HG21	1:21:A:TYR:HA	4	0.18	0.05	0.18
(2,2372)	1:34:A:ILE:HG22	1:21:A:TYR:HA	4	0.18	0.05	0.18
(2,185)	1:20:A:GLU:H	1:36:A:LEU:H	4	0.18	0.02	0.18
(2,185)	1:35:A:ARG:HE	1:36:A:LEU:H	4	0.18	0.02	0.18
(2,3108)	1:42:A:HIS:HA	1:43:A:GLU:HB2	4	0.16	0.02	0.16
(2,1717)	1:49:A:VAL:HB	1:24:A:ILE:HA	4	0.15	0.03	0.15
(2,1273)	1:115:A:TYR:HD2	1:53:A:SER:H	4	0.14	0.05	0.12
(2,1273)	1:115:A:TYR:HD1	1:53:A:SER:H	4	0.14	0.05	0.12
(2,554)	1:71:A:ILE:HG21	1:80:A:PHE:H	4	0.14	0.0	0.14
(2,554)	1:71:A:ILE:HG23	1:80:A:PHE:H	4	0.14	0.0	0.14
(2,554)	1:71:A:ILE:HG22	1:80:A:PHE:H	4	0.14	0.0	0.14
(2,1828)	1:125:A:PRO:HB2	1:125:A:PRO:HA	4	0.14	0.01	0.14
(2,1819)	1:105:A:ASN:HB2	1:106:A:VAL:HA	4	0.13	0.01	0.13
(2,1819)	1:105:A:ASN:HB3	1:106:A:VAL:HA	4	0.13	0.01	0.13
(2,1611)	1:86:A:TRP:HD1	1:84:A:GLU:H	4	0.13	0.02	0.12
(2,1196)	1:45:A:LYS:HB2	1:47:A:ASP:H	4	0.12	0.03	0.12
(2,205)	1:90:A:ALA:HA	1:93:A:ILE:H	4	0.12	0.02	0.11
(2,1714)	1:131:A:GLU:HB2	1:130:A:THR:HB	3	0.65	0.16	0.63
(2,1714)	1:131:A:GLU:HB3	1:130:A:THR:HB	3	0.65	0.16	0.63
(2,863)	1:10:A:LEU:HD12	1:13:A:ILE:H	3	0.48	0.19	0.59

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,863)	1:122:A:ILE:HG22	1:13:A:ILE:H	3	0.48	0.19	0.59
(2,863)	1:122:A:ILE:HG21	1:13:A:ILE:H	3	0.48	0.19	0.59
(2,4249)	1:52:A:LEU:HD11	1:55:A:ARG:HD3	3	0.46	0.13	0.43
(2,4249)	1:52:A:LEU:HD13	1:55:A:ARG:HD3	3	0.46	0.13	0.43
(2,4249)	1:94:A:LEU:HD11	1:55:A:ARG:HD3	3	0.46	0.13	0.43
(2,1894)	1:5:A:ILE:HD11	1:5:A:ILE:HA	3	0.45	0.32	0.25
(2,1894)	1:76:A:ILE:HD13	1:76:A:ILE:HA	3	0.45	0.32	0.25
(2,1894)	1:76:A:ILE:HD11	1:76:A:ILE:HA	3	0.45	0.32	0.25
(2,4136)	1:5:A:ILE:HA	1:5:A:ILE:HD11	3	0.45	0.32	0.25
(2,4136)	1:76:A:ILE:HA	1:76:A:ILE:HD13	3	0.45	0.32	0.25
(2,4136)	1:76:A:ILE:HA	1:76:A:ILE:HD11	3	0.45	0.32	0.25
(2,3799)	1:107:A:ASP:HB3	1:95:A:LEU:HD23	3	0.32	0.11	0.31
(2,3799)	1:107:A:ASP:HB3	1:95:A:LEU:HD22	3	0.32	0.11	0.31
(2,1520)	1:25:A:LYS:HD2	1:62:A:SER:H	3	0.27	0.05	0.27
(2,1520)	1:25:A:LYS:HB3	1:62:A:SER:H	3	0.27	0.05	0.27
(2,1892)	1:8:A:ILE:HG23	1:8:A:ILE:HA	3	0.25	0.02	0.27
(2,1892)	1:8:A:ILE:HG21	1:8:A:ILE:HA	3	0.25	0.02	0.27
(2,3422)	1:71:A:ILE:HA	1:122:A:ILE:HG13	3	0.25	0.06	0.28
(2,4512)	1:121:A:ILE:HD13	1:79:A:TYR:HD1	3	0.24	0.14	0.19
(2,4512)	1:121:A:ILE:HD12	1:79:A:TYR:HD2	3	0.24	0.14	0.19
(2,4264)	1:51:A:LYS:HE2	1:114:A:GLU:HG2	3	0.23	0.13	0.16
(2,4264)	1:101:A:ASN:HB2	1:102:A:VAL:HB	3	0.23	0.13	0.16
(2,1627)	1:135:A:LEU:HD11	1:133:A:THR:H	3	0.22	0.13	0.13
(2,1627)	1:135:A:LEU:HD12	1:133:A:THR:H	3	0.22	0.13	0.13
(2,1627)	1:135:A:LEU:HD13	1:133:A:THR:H	3	0.22	0.13	0.13
(2,3720)	1:86:A:TRP:HH2	1:63:A:LEU:HD22	3	0.21	0.05	0.2
(2,1166)	1:124:A:SER:HB3	1:124:A:SER:H	3	0.2	0.05	0.21
(2,253)	1:22:A:VAL:HG21	1:27:A:ALA:H	3	0.19	0.05	0.19
(2,253)	1:22:A:VAL:HG22	1:27:A:ALA:H	3	0.19	0.05	0.19
(2,4077)	1:90:A:ALA:H	1:56:A:ILE:HD12	3	0.18	0.05	0.16
(2,4077)	1:90:A:ALA:H	1:56:A:ILE:HD13	3	0.18	0.05	0.16
(2,4077)	1:90:A:ALA:H	1:56:A:ILE:HD11	3	0.18	0.05	0.16
(2,2822)	1:118:A:LEU:HB3	1:115:A:TYR:HB2	3	0.16	0.04	0.18
(2,3811)	1:48:A:GLU:HB2	1:49:A:VAL:HG23	3	0.16	0.05	0.17
(2,3811)	1:48:A:GLU:HB2	1:49:A:VAL:HG21	3	0.16	0.05	0.17
(2,2973)	1:109:A:GLU:HA	1:109:A:GLU:HG2	3	0.16	0.03	0.15
(2,1460)	1:9:A:GLY:HA3	1:9:A:GLY:H	3	0.15	0.01	0.15
(2,1025)	1:118:A:LEU:HB2	1:115:A:TYR:H	3	0.13	0.02	0.12
(2,558)	1:104:A:LEU:HD21	1:104:A:LEU:H	3	0.12	0.01	0.12
(2,558)	1:104:A:LEU:HD22	1:104:A:LEU:H	3	0.12	0.01	0.12
(2,558)	1:104:A:LEU:HD23	1:104:A:LEU:H	3	0.12	0.01	0.12
(2,294)	1:127:A:ARG:HA	1:127:A:ARG:H	3	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3784)	1:28:A:LEU:HA	1:32:A:LEU:HD21	3	0.11	0.01	0.11
(2,3784)	1:28:A:LEU:HA	1:32:A:LEU:HD23	3	0.11	0.01	0.11
(2,1870)	1:8:A:ILE:HG12	1:8:A:ILE:HA	3	0.11	0.01	0.1
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG21	3	0.11	0.0	0.11
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG22	3	0.11	0.0	0.11
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG23	3	0.11	0.0	0.11
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG21	3	0.11	0.0	0.11
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG22	3	0.11	0.0	0.11
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG23	3	0.11	0.0	0.11
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG21	3	0.11	0.0	0.11
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG22	3	0.11	0.0	0.11
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG23	3	0.11	0.0	0.11
(2,4536)	1:70:A:PHE:HB2	1:70:A:PHE:HE2	3	0.1	0.0	0.1
(2,4536)	1:70:A:PHE:HB2	1:70:A:PHE:HE1	3	0.1	0.0	0.1
(2,4087)	1:14:A:PHE:HD1	1:13:A:ILE:HD11	2	0.73	0.39	0.73
(2,4087)	1:32:A:LEU:H	1:44:A:ILE:HD11	2	0.73	0.39	0.73
(2,1409)	1:66:A:ILE:HG21	1:87:A:ASN:HD21	2	0.66	0.18	0.66
(2,1409)	1:66:A:ILE:HG22	1:87:A:ASN:HD21	2	0.66	0.18	0.66
(2,4414)	1:132:A:GLU:HG2	1:133:A:THR:HB	2	0.59	0.28	0.59
(2,4414)	1:137:A:GLU:HG2	1:133:A:THR:HB	2	0.59	0.28	0.59
(2,470)	1:53:A:SER:HB3	1:52:A:LEU:H	2	0.57	0.01	0.57
(2,4331)	1:61:A:TRP:HB2	1:24:A:ILE:HD13	2	0.57	0.11	0.57
(2,4331)	1:61:A:TRP:HB2	1:24:A:ILE:HD11	2	0.57	0.11	0.57
(2,4381)	1:133:A:THR:HG21	1:137:A:GLU:HG2	2	0.56	0.14	0.56
(2,4381)	1:130:A:THR:HG22	1:131:A:GLU:HG2	2	0.56	0.14	0.56
(2,3564)	1:55:A:ARG:HD3	1:94:A:LEU:HD12	2	0.5	0.07	0.5
(2,4697)	1:142:A:HIS:HB2	1:142:A:HIS:HD2	2	0.45	0.01	0.45
(2,4697)	1:146:A:HIS:HB3	1:146:A:HIS:HD2	2	0.45	0.01	0.45
(2,3009)	1:34:A:ILE:HG22	1:20:A:GLU:HG2	2	0.44	0.18	0.44
(2,4696)	1:140:A:GLU:HB3	1:141:A:HIS:HD2	2	0.4	0.06	0.4
(2,4696)	1:140:A:GLU:HB3	1:142:A:HIS:HD2	2	0.4	0.06	0.4
(2,1489)	1:8:A:ILE:HG23	1:9:A:GLY:H	2	0.34	0.02	0.34
(2,1489)	1:8:A:ILE:HG21	1:9:A:GLY:H	2	0.34	0.02	0.34
(2,3371)	1:48:A:GLU:H	1:118:A:LEU:HD21	2	0.32	0.04	0.32
(2,3371)	1:48:A:GLU:H	1:118:A:LEU:HD23	2	0.32	0.04	0.32
(2,3354)	1:61:A:TRP:HZ3	1:25:A:LYS:HG2	2	0.3	0.2	0.3
(2,3354)	1:61:A:TRP:HZ3	1:25:A:LYS:HG3	2	0.3	0.2	0.3
(2,2915)	1:115:A:TYR:HD2	1:114:A:GLU:HG2	2	0.3	0.01	0.3
(2,2915)	1:115:A:TYR:HD1	1:114:A:GLU:HG2	2	0.3	0.01	0.3
(2,576)	1:133:A:THR:HG22	1:137:A:GLU:H	2	0.27	0.08	0.27
(2,576)	1:133:A:THR:HG21	1:137:A:GLU:H	2	0.27	0.08	0.27
(2,4468)	1:65:A:LYS:HD2	1:21:A:TYR:HD2	2	0.26	0.07	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4468)	1:35:A:ARG:HB2	1:41:A:TYR:HD2	2	0.26	0.07	0.26
(2,1253)	1:52:A:LEU:HD11	1:56:A:ILE:H	2	0.23	0.11	0.23
(2,974)	1:87:A:ASN:HB3	1:84:A:GLU:H	2	0.22	0.12	0.22
(2,4282)	1:138:A:MET:HA	1:141:A:HIS:HB3	2	0.22	0.07	0.22
(2,2115)	1:36:A:LEU:HB2	1:41:A:TYR:HA	2	0.21	0.08	0.21
(2,2115)	1:33:A:LYS:HG3	1:41:A:TYR:HA	2	0.21	0.08	0.21
(2,4303)	1:89:A:LYS:HD2	1:63:A:LEU:HD11	2	0.2	0.05	0.2
(2,1367)	1:119:A:ILE:HB	1:116:A:THR:H	2	0.18	0.0	0.18
(2,1367)	1:45:A:LYS:HB2	1:116:A:THR:H	2	0.18	0.0	0.18
(2,1016)	1:45:A:LYS:HB3	1:117:A:SER:H	2	0.18	0.08	0.18
(2,4450)	1:132:A:GLU:HB2	1:129:A:TYR:HD1	2	0.18	0.03	0.18
(2,2084)	1:31:A:LYS:HB3	1:22:A:VAL:HA	2	0.16	0.02	0.16
(2,2145)	1:46:A:LYS:HD2	1:46:A:LYS:HA	2	0.16	0.02	0.16
(2,1387)	1:36:A:LEU:HD13	1:16:A:SER:H	2	0.16	0.01	0.16
(2,1387)	1:36:A:LEU:HD11	1:16:A:SER:H	2	0.16	0.01	0.16
(2,3606)	1:56:A:ILE:HG13	1:57:A:PRO:HG3	2	0.16	0.02	0.16
(2,1571)	1:30:A:GLY:H	1:32:A:LEU:H	2	0.16	0.01	0.16
(2,3555)	1:48:A:GLU:HG3	1:118:A:LEU:HD12	2	0.15	0.02	0.15
(2,4705)	1:58:A:LEU:HA	1:61:A:TRP:HZ3	2	0.15	0.01	0.15
(2,4080)	1:28:A:LEU:H	1:24:A:ILE:HG22	2	0.15	0.04	0.15
(2,4080)	1:28:A:LEU:H	1:24:A:ILE:HG23	2	0.15	0.04	0.15
(2,1884)	1:44:A:ILE:HG21	1:117:A:SER:HB3	2	0.15	0.02	0.15
(2,1884)	1:44:A:ILE:HG23	1:117:A:SER:HB3	2	0.15	0.02	0.15
(2,1595)	1:95:A:LEU:HD13	1:107:A:ASP:H	2	0.14	0.02	0.14
(2,1729)	1:52:A:LEU:HG	1:49:A:VAL:HA	2	0.14	0.02	0.14
(2,1735)	1:119:A:ILE:HG23	1:116:A:THR:HA	2	0.14	0.01	0.14
(2,1735)	1:119:A:ILE:HG21	1:116:A:THR:HA	2	0.14	0.01	0.14
(2,2046)	1:91:A:ILE:HA	1:88:A:LYS:HA	2	0.14	0.01	0.14
(2,3971)	1:116:A:THR:HA	1:119:A:ILE:HG23	2	0.14	0.01	0.14
(2,3971)	1:116:A:THR:HA	1:119:A:ILE:HG21	2	0.14	0.01	0.14
(2,195)	1:92:A:SER:HA	1:99:A:ILE:H	2	0.14	0.04	0.14
(2,9)	1:85:A:GLN:HB3	1:86:A:TRP:HE1	2	0.13	0.02	0.13
(2,744)	1:86:A:TRP:HB2	1:87:A:ASN:H	2	0.13	0.01	0.13
(2,1306)	1:19:A:ALA:HA	1:37:A:ASN:HD22	2	0.13	0.0	0.13
(2,1306)	1:15:A:SER:HA	1:37:A:ASN:HD22	2	0.13	0.0	0.13
(2,1324)	1:100:A:SER:HB3	1:101:A:ASN:HD22	2	0.13	0.03	0.13
(2,3434)	1:33:A:LYS:HA	1:34:A:ILE:HG12	2	0.12	0.02	0.12
(2,708)	1:84:A:GLU:HA	1:87:A:ASN:H	2	0.12	0.01	0.12
(2,2173)	1:118:A:LEU:HD12	1:48:A:GLU:HA	2	0.12	0.0	0.12
(2,27)	1:45:A:LYS:HE2	1:46:A:LYS:H	2	0.11	0.0	0.11
(2,27)	1:45:A:LYS:HE3	1:46:A:LYS:H	2	0.11	0.0	0.11
(2,1617)	1:111:A:LEU:HB3	1:115:A:TYR:H	2	0.11	0.0	0.11

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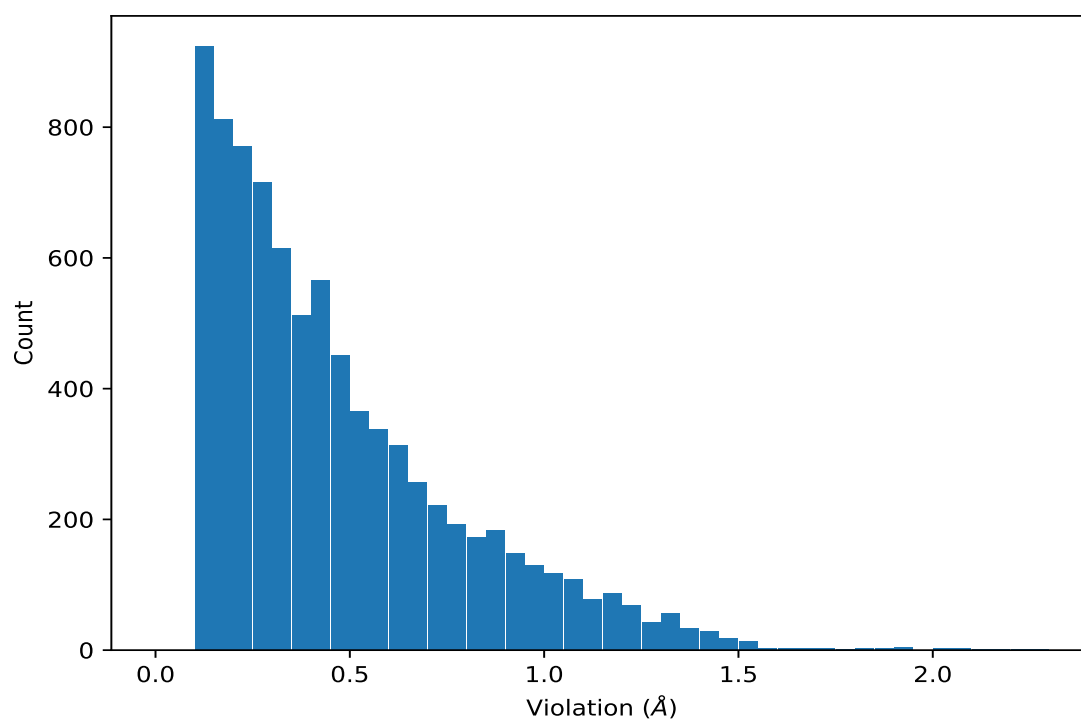
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,808)	1:11:A:LYS:HD2	1:12:A:ASP:H	2	0.11	0.0	0.11
(2,808)	1:11:A:LYS:HD3	1:12:A:ASP:H	2	0.11	0.0	0.11
(2,1629)	1:77:A:GLY:HA2	1:105:A:ASN:HD21	2	0.11	0.0	0.11

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)
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG21	16	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG23	17	2.21
(2,3993)	1:83:A:GLY:HA2	1:66:A:ILE:HG21	10	2.17
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG23	7	2.12
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG21	5	2.05
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG22	18	2.05
(2,3993)	1:83:A:GLY:HA2	1:66:A:ILE:HG21	20	2.05
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG22	3	2.04
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG21	12	2.01
(2,3993)	1:83:A:GLY:HA2	1:66:A:ILE:HG23	2	1.92
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG22	8	1.92
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG21	9	1.92
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG22	13	1.92
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG23	1	1.88
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG21	11	1.86
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG22	13	1.84
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG23	19	1.83
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG23	6	1.82
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB1	8	1.75
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG23	4	1.72
(2,3609)	1:126:A:THR:HG23	1:125:A:PRO:HG2	5	1.71
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG21	18	1.69
(2,3993)	1:83:A:GLY:HA2	1:66:A:ILE:HG21	14	1.69
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG22	9	1.61
(2,1410)	1:119:A:ILE:HG23	1:116:A:THR:H	3	1.6
(2,1404)	1:122:A:ILE:HD13	1:37:A:ASN:HD22	11	1.59
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB1	11	1.58
(2,3993)	1:44:A:ILE:HA	1:66:A:ILE:HG21	15	1.57
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD13	7	1.54
(2,3855)	1:121:A:ILE:HD12	1:108:A:VAL:HG22	13	1.54
(2,1401)	1:106:A:VAL:HG22	1:105:A:ASN:HD22	7	1.54
(2,1071)	1:119:A:ILE:HG22	1:117:A:SER:H	3	1.54
(2,3855)	1:81:A:VAL:HG23	1:108:A:VAL:HG21	18	1.53
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG21	12	1.52
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB3	6	1.52
(2,1071)	1:119:A:ILE:HG23	1:117:A:SER:H	20	1.52
(2,1404)	1:122:A:ILE:HD11	1:37:A:ASN:HD22	7	1.51
(2,1071)	1:119:A:ILE:HG23	1:117:A:SER:H	6	1.51
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG21	15	1.5
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB1	16	1.5
(2,1075)	1:119:A:ILE:HG21	1:115:A:TYR:H	20	1.5
(2,1071)	1:119:A:ILE:HG22	1:117:A:SER:H	10	1.5
(2,3855)	1:121:A:ILE:HD13	1:108:A:VAL:HG23	11	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1075)	1:52:A:LEU:HD11	1:115:A:TYR:H	5	1.49
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG21	7	1.48
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG21	14	1.48
(2,3855)	1:121:A:ILE:HD13	1:108:A:VAL:HG21	6	1.48
(2,1412)	1:108:A:VAL:HG13	1:114:A:GLU:H	18	1.48
(2,1410)	1:119:A:ILE:HG21	1:116:A:THR:H	20	1.48
(2,1075)	1:119:A:ILE:HG23	1:115:A:TYR:H	12	1.48
(2,1075)	1:119:A:ILE:HG23	1:115:A:TYR:H	18	1.48
(2,3855)	1:121:A:ILE:HD13	1:108:A:VAL:HG22	10	1.47
(2,1410)	1:119:A:ILE:HG21	1:116:A:THR:H	6	1.46
(2,1071)	1:119:A:ILE:HG23	1:117:A:SER:H	9	1.46
(2,889)	1:91:A:ILE:HD11	1:87:A:ASN:H	17	1.46
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG22	11	1.45
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG22	15	1.45
(2,3855)	1:121:A:ILE:HD12	1:108:A:VAL:HG22	2	1.45
(2,3271)	1:28:A:LEU:HD11	1:25:A:LYS:HD3	3	1.45
(2,1410)	1:119:A:ILE:HG23	1:116:A:THR:H	10	1.45
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD12	4	1.44
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG21	17	1.44
(2,3855)	1:81:A:VAL:HG21	1:108:A:VAL:HG21	3	1.44
(2,3794)	1:124:A:SER:HB2	1:126:A:THR:HG23	19	1.44
(2,1071)	1:119:A:ILE:HG23	1:117:A:SER:H	1	1.44
(2,889)	1:91:A:ILE:HD13	1:87:A:ASN:H	1	1.44
(2,1075)	1:119:A:ILE:HG23	1:115:A:TYR:H	2	1.43
(2,1071)	1:119:A:ILE:HG22	1:117:A:SER:H	7	1.43
(2,1071)	1:119:A:ILE:HG22	1:117:A:SER:H	18	1.43
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD12	18	1.42
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG23	6	1.42
(2,3855)	1:81:A:VAL:HG22	1:108:A:VAL:HG22	14	1.42
(2,2197)	1:24:A:ILE:HG22	1:62:A:SER:HA	20	1.42
(2,1410)	1:119:A:ILE:HG23	1:116:A:THR:H	18	1.42
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB3	2	1.41
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB2	3	1.41
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB1	20	1.41
(2,1401)	1:106:A:VAL:HG23	1:105:A:ASN:HD22	2	1.41
(2,1071)	1:119:A:ILE:HG21	1:117:A:SER:H	4	1.41
(2,4161)	1:70:A:PHE:HB2	1:71:A:ILE:HD11	3	1.4
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD11	9	1.4
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD13	1	1.4
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB3	1	1.4
(2,3855)	1:121:A:ILE:HD11	1:108:A:VAL:HG23	7	1.4
(2,1410)	1:119:A:ILE:HG22	1:116:A:THR:H	5	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1410)	1:119:A:ILE:HG23	1:116:A:THR:H	12	1.4
(2,1401)	1:106:A:VAL:HG23	1:105:A:ASN:HD22	6	1.4
(2,1071)	1:119:A:ILE:HG22	1:117:A:SER:H	2	1.4
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD13	14	1.39
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG22	8	1.39
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	3	1.39
(2,1410)	1:119:A:ILE:HG22	1:116:A:THR:H	4	1.39
(2,889)	1:91:A:ILE:HD11	1:87:A:ASN:H	10	1.39
(2,3855)	1:121:A:ILE:HD11	1:108:A:VAL:HG23	8	1.38
(2,1075)	1:119:A:ILE:HG21	1:115:A:TYR:H	9	1.38
(2,1071)	1:119:A:ILE:HG22	1:117:A:SER:H	11	1.38
(2,889)	1:63:A:LEU:HD22	1:87:A:ASN:H	11	1.38
(2,4384)	1:34:A:ILE:HG21	1:33:A:LYS:HB3	5	1.37
(2,1410)	1:119:A:ILE:HG23	1:116:A:THR:H	2	1.37
(2,1075)	1:52:A:LEU:HD11	1:115:A:TYR:H	3	1.37
(2,1071)	1:119:A:ILE:HG22	1:117:A:SER:H	12	1.37
(2,1071)	1:119:A:ILE:HG21	1:117:A:SER:H	15	1.37
(2,889)	1:91:A:ILE:HD11	1:87:A:ASN:H	9	1.37
(2,889)	1:91:A:ILE:HD12	1:87:A:ASN:H	14	1.37
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD12	6	1.36
(2,3855)	1:81:A:VAL:HG22	1:108:A:VAL:HG22	15	1.36
(2,1652)	1:111:A:LEU:HD11	1:110:A:LYS:H	8	1.36
(2,1412)	1:94:A:LEU:HD12	1:114:A:GLU:H	3	1.36
(2,1410)	1:119:A:ILE:HG21	1:116:A:THR:H	1	1.36
(2,1075)	1:119:A:ILE:HG23	1:115:A:TYR:H	10	1.36
(2,1071)	1:119:A:ILE:HG21	1:117:A:SER:H	5	1.36
(2,889)	1:91:A:ILE:HD13	1:87:A:ASN:H	15	1.36
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD11	6	1.35
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD13	4	1.35
(2,3855)	1:121:A:ILE:HD11	1:108:A:VAL:HG21	1	1.35
(2,3855)	1:81:A:VAL:HG21	1:108:A:VAL:HG23	4	1.35
(2,1412)	1:119:A:ILE:HG21	1:114:A:GLU:H	1	1.35
(2,1410)	1:52:A:LEU:HD21	1:116:A:THR:H	7	1.35
(2,1410)	1:119:A:ILE:HG21	1:116:A:THR:H	9	1.35
(2,1075)	1:119:A:ILE:HG21	1:115:A:TYR:H	6	1.35
(2,1071)	1:119:A:ILE:HG23	1:117:A:SER:H	19	1.35
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD12	2	1.34
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG22	3	1.34
(2,3855)	1:121:A:ILE:HD11	1:108:A:VAL:HG23	17	1.34
(2,1652)	1:111:A:LEU:HD13	1:110:A:LYS:H	9	1.34
(2,1404)	1:122:A:ILE:HD12	1:37:A:ASN:HD22	20	1.34
(2,1399)	1:56:A:ILE:HG22	1:55:A:ARG:HE	6	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,889)	1:63:A:LEU:HD23	1:87:A:ASN:H	5	1.34
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD11	7	1.33
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB1	7	1.33
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG23	19	1.33
(2,3855)	1:121:A:ILE:HD12	1:108:A:VAL:HG22	20	1.33
(2,2197)	1:24:A:ILE:HG22	1:62:A:SER:HA	17	1.33
(2,1412)	1:94:A:LEU:HD13	1:114:A:GLU:H	2	1.33
(2,1412)	1:94:A:LEU:HD11	1:114:A:GLU:H	20	1.33
(2,1410)	1:119:A:ILE:HG23	1:116:A:THR:H	11	1.33
(2,1401)	1:106:A:VAL:HG23	1:105:A:ASN:HD22	15	1.33
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD13	13	1.32
(2,4161)	1:70:A:PHE:HB2	1:71:A:ILE:HD13	14	1.32
(2,2197)	1:24:A:ILE:HG23	1:62:A:SER:HA	14	1.32
(2,2197)	1:24:A:ILE:HG23	1:62:A:SER:HA	18	1.32
(2,1412)	1:119:A:ILE:HG21	1:114:A:GLU:H	19	1.32
(2,1410)	1:119:A:ILE:HG22	1:116:A:THR:H	15	1.32
(2,1401)	1:106:A:VAL:HG21	1:105:A:ASN:HD22	20	1.32
(2,1075)	1:119:A:ILE:HG21	1:115:A:TYR:H	19	1.32
(2,4384)	1:34:A:ILE:HG21	1:33:A:LYS:HB3	1	1.31
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD13	3	1.31
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD13	8	1.31
(2,4161)	1:70:A:PHE:HB2	1:71:A:ILE:HD12	4	1.31
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG21	4	1.31
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG22	16	1.31
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG21	20	1.31
(2,3855)	1:121:A:ILE:HD12	1:108:A:VAL:HG23	9	1.31
(2,3794)	1:124:A:SER:HB3	1:126:A:THR:HG22	4	1.31
(2,1652)	1:112:A:LEU:HD11	1:110:A:LYS:H	19	1.31
(2,1638)	1:24:A:ILE:HG22	1:62:A:SER:H	17	1.31
(2,1412)	1:119:A:ILE:HG21	1:114:A:GLU:H	9	1.31
(2,1412)	1:119:A:ILE:HG23	1:114:A:GLU:H	10	1.31
(2,1412)	1:108:A:VAL:HG12	1:114:A:GLU:H	12	1.31
(2,1075)	1:119:A:ILE:HG22	1:115:A:TYR:H	4	1.31
(2,889)	1:91:A:ILE:HD12	1:87:A:ASN:H	6	1.31
(2,4384)	1:34:A:ILE:HG22	1:33:A:LYS:HB3	9	1.3
(2,4384)	1:34:A:ILE:HG21	1:33:A:LYS:HB3	14	1.3
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD12	13	1.3
(2,4161)	1:70:A:PHE:HB2	1:71:A:ILE:HD11	2	1.3
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD12	13	1.3
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG23	9	1.3
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG22	5	1.3
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG22	13	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD23	9	1.3
(2,2197)	1:24:A:ILE:HG22	1:62:A:SER:HA	4	1.3
(2,2197)	1:24:A:ILE:HG22	1:62:A:SER:HA	10	1.3
(2,1638)	1:24:A:ILE:HG23	1:62:A:SER:H	1	1.3
(2,1638)	1:24:A:ILE:HG21	1:62:A:SER:H	18	1.3
(2,1412)	1:119:A:ILE:HG23	1:114:A:GLU:H	7	1.3
(2,1402)	1:99:A:ILE:HG21	1:101:A:ASN:HD22	12	1.3
(2,1075)	1:119:A:ILE:HG21	1:115:A:TYR:H	1	1.3
(2,4384)	1:34:A:ILE:HG21	1:33:A:LYS:HB3	8	1.29
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD13	20	1.29
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD11	9	1.29
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD12	11	1.29
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD21	4	1.29
(2,1652)	1:111:A:LEU:HD11	1:110:A:LYS:H	5	1.29
(2,1638)	1:24:A:ILE:HG23	1:62:A:SER:H	4	1.29
(2,1638)	1:24:A:ILE:HG23	1:62:A:SER:H	14	1.29
(2,889)	1:91:A:ILE:HD13	1:87:A:ASN:H	12	1.29
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB2	12	1.28
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB2	8	1.28
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB3	18	1.28
(2,3838)	1:31:A:LYS:HG2	1:22:A:VAL:HG12	3	1.28
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD12	19	1.27
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB2	16	1.27
(2,3855)	1:81:A:VAL:HG23	1:108:A:VAL:HG23	12	1.27
(2,3855)	1:121:A:ILE:HD13	1:108:A:VAL:HG21	19	1.27
(2,2377)	1:52:A:LEU:HD23	1:115:A:TYR:HA	15	1.27
(2,1638)	1:24:A:ILE:HG21	1:62:A:SER:H	6	1.27
(2,1412)	1:94:A:LEU:HD13	1:114:A:GLU:H	5	1.27
(2,1401)	1:106:A:VAL:HG23	1:105:A:ASN:HD22	5	1.27
(2,889)	1:63:A:LEU:HD22	1:87:A:ASN:H	20	1.27
(2,560)	1:95:A:LEU:HD13	1:104:A:LEU:H	7	1.27
(2,4384)	1:34:A:ILE:HG22	1:33:A:LYS:HB3	16	1.26
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD12	3	1.26
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD13	7	1.26
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB2	9	1.26
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB3	13	1.26
(2,1652)	1:111:A:LEU:HD11	1:110:A:LYS:H	13	1.26
(2,1410)	1:119:A:ILE:HG21	1:116:A:THR:H	19	1.26
(2,1401)	1:106:A:VAL:HG21	1:105:A:ASN:HD22	16	1.26
(2,889)	1:91:A:ILE:HD13	1:87:A:ASN:H	16	1.26
(2,889)	1:91:A:ILE:HD12	1:87:A:ASN:H	19	1.26
(2,344)	1:108:A:VAL:HG13	1:71:A:ILE:H	16	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD11	1	1.25
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG22	19	1.25
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB1	4	1.25
(2,3855)	1:121:A:ILE:HD11	1:108:A:VAL:HG23	5	1.25
(2,3855)	1:121:A:ILE:HD12	1:108:A:VAL:HG23	16	1.25
(2,2377)	1:52:A:LEU:HD21	1:115:A:TYR:HA	10	1.25
(2,2197)	1:24:A:ILE:HG22	1:62:A:SER:HA	2	1.25
(2,1638)	1:24:A:ILE:HG23	1:62:A:SER:H	20	1.25
(2,889)	1:91:A:ILE:HD11	1:87:A:ASN:H	18	1.25
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD11	5	1.24
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD13	9	1.24
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD13	20	1.24
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD11	6	1.24
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD11	13	1.24
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD13	12	1.24
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB2	3	1.24
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB1	5	1.24
(2,2197)	1:24:A:ILE:HG21	1:62:A:SER:HA	6	1.24
(2,1412)	1:119:A:ILE:HG21	1:114:A:GLU:H	16	1.24
(2,1071)	1:119:A:ILE:HG23	1:117:A:SER:H	14	1.24
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD12	2	1.23
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD11	17	1.23
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD13	5	1.23
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD12	16	1.23
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD13	1	1.23
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD11	6	1.23
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD12	13	1.23
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG21	2	1.23
(2,3794)	1:124:A:SER:HB3	1:126:A:THR:HG23	7	1.23
(2,2197)	1:24:A:ILE:HG23	1:62:A:SER:HA	1	1.23
(2,1412)	1:119:A:ILE:HG22	1:114:A:GLU:H	17	1.23
(2,1392)	1:119:A:ILE:HD11	1:116:A:THR:H	3	1.23
(2,889)	1:91:A:ILE:HD13	1:87:A:ASN:H	7	1.23
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD11	10	1.22
(2,4190)	1:64:A:VAL:HG23	1:24:A:ILE:HG23	5	1.22
(2,4190)	1:64:A:VAL:HG23	1:24:A:ILE:HG23	8	1.22
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD11	8	1.22
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD11	15	1.22
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD13	19	1.22
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD13	8	1.22
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD12	5	1.22
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB1	10	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD23	17	1.22
(2,2377)	1:52:A:LEU:HD12	1:115:A:TYR:HA	18	1.22
(2,1885)	1:123:A:LEU:HD23	1:125:A:PRO:HA	7	1.22
(2,1399)	1:56:A:ILE:HG21	1:55:A:ARG:HE	18	1.22
(2,1075)	1:119:A:ILE:HG22	1:115:A:TYR:H	15	1.22
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	18	1.22
(2,4384)	1:34:A:ILE:HG23	1:33:A:LYS:HB3	10	1.21
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD13	8	1.21
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD12	11	1.21
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD13	9	1.21
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD11	17	1.21
(2,2377)	1:52:A:LEU:HD23	1:115:A:TYR:HA	20	1.21
(2,2197)	1:24:A:ILE:HG22	1:62:A:SER:HA	7	1.21
(2,2197)	1:24:A:ILE:HG23	1:62:A:SER:HA	16	1.21
(2,1652)	1:112:A:LEU:HD11	1:110:A:LYS:H	11	1.21
(2,1638)	1:24:A:ILE:HG23	1:62:A:SER:H	7	1.21
(2,1392)	1:119:A:ILE:HD12	1:116:A:THR:H	6	1.21
(2,1071)	1:119:A:ILE:HG21	1:117:A:SER:H	13	1.21
(2,889)	1:91:A:ILE:HD12	1:87:A:ASN:H	8	1.21
(2,344)	1:108:A:VAL:HG13	1:71:A:ILE:H	9	1.21
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD12	15	1.2
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD12	19	1.2
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD12	10	1.2
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD12	15	1.2
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD11	2	1.2
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD11	11	1.2
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD11	19	1.2
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD22	10	1.2
(2,2377)	1:52:A:LEU:HD21	1:115:A:TYR:HA	9	1.2
(2,2197)	1:24:A:ILE:HG23	1:62:A:SER:HA	12	1.2
(2,2197)	1:24:A:ILE:HG23	1:62:A:SER:HA	15	1.2
(2,1652)	1:112:A:LEU:HD13	1:110:A:LYS:H	2	1.2
(2,1652)	1:95:A:LEU:HD12	1:110:A:LYS:H	7	1.2
(2,1392)	1:119:A:ILE:HD12	1:116:A:THR:H	20	1.2
(2,344)	1:119:A:ILE:HG23	1:71:A:ILE:H	5	1.2
(2,4384)	1:34:A:ILE:HG22	1:33:A:LYS:HB3	7	1.19
(2,4384)	1:34:A:ILE:HG22	1:33:A:LYS:HB3	11	1.19
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD12	12	1.19
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG23	1	1.19
(2,3922)	1:68:A:PHE:HE1	1:56:A:ILE:HG22	18	1.19
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG22	20	1.19
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD23	2	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG21	14	1.19
(2,3243)	1:56:A:ILE:HD11	1:61:A:TRP:HB2	12	1.19
(2,2197)	1:24:A:ILE:HG23	1:62:A:SER:HA	3	1.19
(2,2197)	1:24:A:ILE:HG23	1:62:A:SER:HA	13	1.19
(2,1652)	1:112:A:LEU:HD13	1:110:A:LYS:H	12	1.19
(2,1638)	1:24:A:ILE:HG21	1:62:A:SER:H	3	1.19
(2,1638)	1:24:A:ILE:HG23	1:62:A:SER:H	8	1.19
(2,1638)	1:24:A:ILE:HG21	1:62:A:SER:H	16	1.19
(2,1399)	1:56:A:ILE:HG23	1:55:A:ARG:HE	10	1.19
(2,1075)	1:119:A:ILE:HG22	1:115:A:TYR:H	8	1.19
(2,4689)	1:123:A:LEU:HD22	1:79:A:TYR:HD2	7	1.18
(2,4384)	1:34:A:ILE:HG22	1:33:A:LYS:HB3	19	1.18
(2,4384)	1:34:A:ILE:HG22	1:33:A:LYS:HB3	20	1.18
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD13	3	1.18
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD12	10	1.18
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD11	18	1.18
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD12	16	1.18
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB1	11	1.18
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB2	14	1.18
(2,2377)	1:52:A:LEU:HD21	1:115:A:TYR:HA	12	1.18
(2,2197)	1:24:A:ILE:HG22	1:62:A:SER:HA	5	1.18
(2,1638)	1:24:A:ILE:HG21	1:62:A:SER:H	15	1.18
(2,1412)	1:94:A:LEU:HD12	1:114:A:GLU:H	4	1.18
(2,1392)	1:119:A:ILE:HD13	1:116:A:THR:H	4	1.18
(2,1392)	1:119:A:ILE:HD11	1:116:A:THR:H	10	1.18
(2,4300)	1:59:A:TYR:HB2	1:63:A:LEU:HD21	4	1.17
(2,4161)	1:89:A:LYS:HE2	1:93:A:ILE:HD12	18	1.17
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD12	19	1.17
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD13	20	1.17
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD12	11	1.17
(2,1652)	1:112:A:LEU:HD12	1:110:A:LYS:H	6	1.17
(2,1638)	1:24:A:ILE:HG23	1:62:A:SER:H	10	1.17
(2,1638)	1:24:A:ILE:HG21	1:62:A:SER:H	12	1.17
(2,1412)	1:119:A:ILE:HG21	1:114:A:GLU:H	6	1.17
(2,1410)	1:119:A:ILE:HG22	1:116:A:THR:H	8	1.17
(2,1075)	1:119:A:ILE:HG22	1:115:A:TYR:H	17	1.17
(2,1071)	1:119:A:ILE:HG21	1:117:A:SER:H	8	1.17
(2,889)	1:91:A:ILE:HD13	1:87:A:ASN:H	4	1.17
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	20	1.17
(2,344)	1:108:A:VAL:HG12	1:71:A:ILE:H	17	1.17
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD13	4	1.16
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD13	15	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD12	10	1.16
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD11	18	1.16
(2,4084)	1:56:A:ILE:H	1:93:A:ILE:HD13	10	1.16
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG22	8	1.16
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD12	12	1.16
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD11	14	1.16
(2,2377)	1:52:A:LEU:HD13	1:115:A:TYR:HA	2	1.16
(2,1833)	1:132:A:GLU:HB2	1:133:A:THR:HA	18	1.16
(2,1652)	1:112:A:LEU:HD11	1:110:A:LYS:H	1	1.16
(2,1652)	1:112:A:LEU:HD12	1:110:A:LYS:H	18	1.16
(2,1638)	1:24:A:ILE:HG23	1:62:A:SER:H	9	1.16
(2,1410)	1:119:A:ILE:HG22	1:116:A:THR:H	13	1.16
(2,889)	1:91:A:ILE:HD12	1:87:A:ASN:H	2	1.16
(2,867)	1:64:A:VAL:HG13	1:88:A:LYS:H	2	1.16
(2,867)	1:64:A:VAL:HG13	1:88:A:LYS:H	16	1.16
(2,4384)	1:34:A:ILE:HG23	1:33:A:LYS:HB3	13	1.15
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD12	1	1.15
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD11	7	1.15
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD11	12	1.15
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD11	9	1.15
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD12	18	1.15
(2,4122)	1:22:A:VAL:HA	1:66:A:ILE:HD12	13	1.15
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD12	17	1.15
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD11	12	1.15
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD12	5	1.15
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB3	9	1.15
(2,3838)	1:31:A:LYS:HG2	1:22:A:VAL:HG12	16	1.15
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD22	18	1.15
(2,3681)	1:75:A:GLU:H	1:126:A:THR:HG21	16	1.15
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD12	6	1.15
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD13	13	1.15
(2,3243)	1:63:A:LEU:HB2	1:61:A:TRP:HB2	2	1.15
(2,1638)	1:24:A:ILE:HG23	1:62:A:SER:H	2	1.15
(2,1638)	1:24:A:ILE:HG23	1:62:A:SER:H	5	1.15
(2,1638)	1:24:A:ILE:HG21	1:62:A:SER:H	11	1.15
(2,1638)	1:24:A:ILE:HG21	1:62:A:SER:H	13	1.15
(2,1410)	1:119:A:ILE:HG21	1:116:A:THR:H	14	1.15
(2,344)	1:108:A:VAL:HG12	1:71:A:ILE:H	19	1.15
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD11	14	1.14
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD12	1	1.14
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD11	4	1.14
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD13	15	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD12	6	1.14
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD12	14	1.14
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB1	7	1.14
(2,3838)	1:31:A:LYS:HG2	1:22:A:VAL:HG12	1	1.14
(2,3838)	1:31:A:LYS:HG2	1:22:A:VAL:HG13	4	1.14
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD23	12	1.14
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG21	7	1.14
(2,3243)	1:56:A:ILE:HD12	1:61:A:TRP:HB2	19	1.14
(2,2373)	1:36:A:LEU:HD22	1:21:A:TYR:HA	15	1.14
(2,2197)	1:24:A:ILE:HG23	1:62:A:SER:HA	11	1.14
(2,1652)	1:112:A:LEU:HD13	1:110:A:LYS:H	4	1.14
(2,1412)	1:119:A:ILE:HG22	1:114:A:GLU:H	15	1.14
(2,1402)	1:99:A:ILE:HG22	1:101:A:ASN:HD22	1	1.14
(2,4161)	1:89:A:LYS:HE3	1:93:A:ILE:HD13	5	1.13
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD11	5	1.13
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD12	11	1.13
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD11	6	1.13
(2,3922)	1:68:A:PHE:HE2	1:56:A:ILE:HG21	10	1.13
(2,2377)	1:52:A:LEU:HD13	1:115:A:TYR:HA	16	1.13
(2,2197)	1:24:A:ILE:HG22	1:62:A:SER:HA	8	1.13
(2,2197)	1:24:A:ILE:HG23	1:62:A:SER:HA	9	1.13
(2,1412)	1:119:A:ILE:HG22	1:114:A:GLU:H	8	1.13
(2,1392)	1:119:A:ILE:HD11	1:116:A:THR:H	2	1.13
(2,1392)	1:119:A:ILE:HD11	1:116:A:THR:H	9	1.13
(2,1392)	1:119:A:ILE:HD12	1:116:A:THR:H	12	1.13
(2,761)	1:107:A:ASP:HB3	1:103:A:ILE:H	8	1.13
(2,761)	1:107:A:ASP:HB3	1:103:A:ILE:H	9	1.13
(2,344)	1:108:A:VAL:HG13	1:71:A:ILE:H	6	1.13
(2,344)	1:108:A:VAL:HG12	1:71:A:ILE:H	8	1.13
(2,4384)	1:34:A:ILE:HG21	1:33:A:LYS:HB3	4	1.12
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD13	12	1.12
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD11	14	1.12
(2,4190)	1:64:A:VAL:HG23	1:24:A:ILE:HG21	13	1.12
(2,4122)	1:22:A:VAL:HA	1:66:A:ILE:HD12	9	1.12
(2,4087)	1:32:A:LEU:H	1:44:A:ILE:HD11	11	1.12
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD11	18	1.12
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB3	12	1.12
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG23	17	1.12
(2,2873)	1:91:A:ILE:HD11	1:87:A:ASN:HB2	17	1.12
(2,2377)	1:52:A:LEU:HD13	1:115:A:TYR:HA	11	1.12
(2,1652)	1:112:A:LEU:HD11	1:110:A:LYS:H	10	1.12
(2,1075)	1:119:A:ILE:HG23	1:115:A:TYR:H	11	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1071)	1:119:A:ILE:HG21	1:117:A:SER:H	17	1.12
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	2	1.12
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD1	7	1.11
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD12	16	1.11
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD13	12	1.11
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD13	14	1.11
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD11	10	1.11
(2,3243)	1:56:A:ILE:HD11	1:61:A:TRP:HB2	6	1.11
(2,3243)	1:63:A:LEU:HB2	1:61:A:TRP:HB2	17	1.11
(2,2873)	1:91:A:ILE:HD13	1:87:A:ASN:HB2	1	1.11
(2,2197)	1:24:A:ILE:HG21	1:62:A:SER:HA	19	1.11
(2,1410)	1:119:A:ILE:HG22	1:116:A:THR:H	17	1.11
(2,1404)	1:122:A:ILE:HD11	1:37:A:ASN:HD22	19	1.11
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	17	1.11
(2,600)	1:91:A:ILE:HD13	1:69:A:ILE:H	12	1.11
(2,4384)	1:34:A:ILE:HG23	1:33:A:LYS:HB3	12	1.1
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD12	2	1.1
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD11	10	1.1
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD12	11	1.1
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD13	7	1.1
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD12	3	1.1
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD23	1	1.1
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD23	20	1.1
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD12	17	1.1
(2,3243)	1:56:A:ILE:HD13	1:61:A:TRP:HB2	18	1.1
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	2	1.1
(2,1399)	1:93:A:ILE:HG21	1:55:A:ARG:HE	12	1.1
(2,1392)	1:119:A:ILE:HD13	1:116:A:THR:H	7	1.1
(2,1392)	1:119:A:ILE:HD13	1:116:A:THR:H	18	1.1
(2,867)	1:64:A:VAL:HG11	1:88:A:LYS:H	10	1.1
(2,761)	1:107:A:ASP:HB3	1:103:A:ILE:H	15	1.1
(2,168)	1:119:A:ILE:HG23	1:122:A:ILE:H	14	1.1
(2,4190)	1:64:A:VAL:HG22	1:24:A:ILE:HG21	15	1.09
(2,4122)	1:22:A:VAL:HA	1:66:A:ILE:HD11	1	1.09
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD13	4	1.09
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD12	20	1.09
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG23	1	1.09
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD12	4	1.09
(2,3243)	1:63:A:LEU:HB2	1:61:A:TRP:HB2	4	1.09
(2,3243)	1:63:A:LEU:HB2	1:61:A:TRP:HB2	8	1.09
(2,2652)	1:95:A:LEU:HD22	1:107:A:ASP:HB2	13	1.09
(2,2377)	1:52:A:LEU:HD13	1:115:A:TYR:HA	1	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	18	1.09
(2,1652)	1:112:A:LEU:HD12	1:110:A:LYS:H	15	1.09
(2,1392)	1:119:A:ILE:HD12	1:116:A:THR:H	1	1.09
(2,1075)	1:119:A:ILE:HG21	1:115:A:TYR:H	16	1.09
(2,867)	1:64:A:VAL:HG13	1:88:A:LYS:H	6	1.09
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	14	1.09
(2,344)	1:108:A:VAL:HG13	1:71:A:ILE:H	10	1.09
(2,344)	1:108:A:VAL:HG12	1:71:A:ILE:H	13	1.09
(2,168)	1:119:A:ILE:HG23	1:122:A:ILE:H	20	1.09
(2,4384)	1:34:A:ILE:HG23	1:33:A:LYS:HB3	3	1.08
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD12	18	1.08
(2,4300)	1:65:A:LYS:HE3	1:63:A:LEU:HD23	1	1.08
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD11	17	1.08
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD12	12	1.08
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD11	10	1.08
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB3	2	1.08
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG22	4	1.08
(2,3243)	1:63:A:LEU:HB2	1:61:A:TRP:HB2	5	1.08
(2,3243)	1:56:A:ILE:HD12	1:61:A:TRP:HB2	13	1.08
(2,3243)	1:56:A:ILE:HD12	1:61:A:TRP:HB2	16	1.08
(2,2338)	1:67:A:PRO:HG3	1:21:A:TYR:HA	19	1.08
(2,1652)	1:112:A:LEU:HD13	1:110:A:LYS:H	14	1.08
(2,1652)	1:112:A:LEU:HD13	1:110:A:LYS:H	20	1.08
(2,1643)	1:91:A:ILE:HG21	1:93:A:ILE:H	9	1.08
(2,1643)	1:91:A:ILE:HG21	1:93:A:ILE:H	13	1.08
(2,1404)	1:35:A:ARG:HG2	1:37:A:ASN:HD22	18	1.08
(2,1401)	1:106:A:VAL:HG22	1:105:A:ASN:HD22	1	1.08
(2,1392)	1:119:A:ILE:HD11	1:116:A:THR:H	5	1.08
(2,1392)	1:119:A:ILE:HD11	1:116:A:THR:H	11	1.08
(2,867)	1:99:A:ILE:HG22	1:88:A:LYS:H	8	1.08
(2,4518)	1:102:A:VAL:HG23	1:80:A:PHE:HZ	6	1.07
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE2	13	1.07
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD12	6	1.07
(2,4209)	1:68:A:PHE:HA	1:91:A:ILE:HD12	20	1.07
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG23	5	1.07
(2,4105)	1:59:A:TYR:HE1	1:93:A:ILE:HD12	1	1.07
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD23	11	1.07
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD12	16	1.07
(2,3243)	1:56:A:ILE:HD12	1:61:A:TRP:HB2	10	1.07
(2,2873)	1:91:A:ILE:HD12	1:87:A:ASN:HB2	20	1.07
(2,2338)	1:67:A:PRO:HG3	1:21:A:TYR:HA	11	1.07
(2,1392)	1:119:A:ILE:HD12	1:116:A:THR:H	15	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,889)	1:91:A:ILE:HD12	1:87:A:ASN:H	13	1.07
(2,867)	1:99:A:ILE:HG22	1:88:A:LYS:H	19	1.07
(2,560)	1:95:A:LEU:HD13	1:104:A:LEU:H	13	1.07
(2,4384)	1:34:A:ILE:HG22	1:33:A:LYS:HB3	17	1.06
(2,4209)	1:68:A:PHE:HA	1:91:A:ILE:HD13	15	1.06
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD12	12	1.06
(2,4092)	1:14:A:PHE:HD2	1:122:A:ILE:HD11	9	1.06
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD11	17	1.06
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD13	1	1.06
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD21	14	1.06
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG21	2	1.06
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD12	1	1.06
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD13	3	1.06
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD13	11	1.06
(2,3243)	1:63:A:LEU:HB2	1:61:A:TRP:HB2	1	1.06
(2,3111)	1:21:A:TYR:HA	1:65:A:LYS:HD3	2	1.06
(2,2873)	1:91:A:ILE:HD12	1:87:A:ASN:HB2	5	1.06
(2,2652)	1:104:A:LEU:HD23	1:107:A:ASP:HB2	7	1.06
(2,2377)	1:52:A:LEU:HD11	1:115:A:TYR:HA	8	1.06
(2,2377)	1:52:A:LEU:HD12	1:115:A:TYR:HA	14	1.06
(2,2373)	1:36:A:LEU:HD23	1:21:A:TYR:HA	17	1.06
(2,2338)	1:65:A:LYS:HD3	1:21:A:TYR:HA	2	1.06
(2,1652)	1:112:A:LEU:HD13	1:110:A:LYS:H	3	1.06
(2,1652)	1:112:A:LEU:HD12	1:110:A:LYS:H	17	1.06
(2,1643)	1:91:A:ILE:HG22	1:93:A:ILE:H	1	1.06
(2,1075)	1:119:A:ILE:HG21	1:115:A:TYR:H	14	1.06
(2,1071)	1:119:A:ILE:HG23	1:117:A:SER:H	16	1.06
(2,560)	1:95:A:LEU:HD13	1:104:A:LEU:H	8	1.06
(2,344)	1:108:A:VAL:HG11	1:71:A:ILE:H	1	1.06
(2,4518)	1:76:A:ILE:HD13	1:80:A:PHE:HZ	7	1.05
(2,4318)	1:31:A:LYS:HB3	1:27:A:ALA:HB2	6	1.05
(2,4318)	1:31:A:LYS:HB3	1:27:A:ALA:HB3	9	1.05
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD13	9	1.05
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD12	14	1.05
(2,4190)	1:64:A:VAL:HG21	1:24:A:ILE:HG23	7	1.05
(2,4161)	1:70:A:PHE:HB2	1:71:A:ILE:HD13	17	1.05
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD12	19	1.05
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD12	18	1.05
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD13	15	1.05
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD22	12	1.05
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD13	14	1.05
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD12	1	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3243)	1:56:A:ILE:HD13	1:61:A:TRP:HB2	3	1.05
(2,3243)	1:56:A:ILE:HD11	1:61:A:TRP:HB2	11	1.05
(2,3243)	1:56:A:ILE:HD13	1:61:A:TRP:HB2	14	1.05
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	11	1.05
(2,2373)	1:36:A:LEU:HD22	1:21:A:TYR:HA	3	1.05
(2,2373)	1:66:A:ILE:HD12	1:21:A:TYR:HA	13	1.05
(2,2373)	1:36:A:LEU:HD22	1:21:A:TYR:HA	18	1.05
(2,2373)	1:36:A:LEU:HD21	1:21:A:TYR:HA	20	1.05
(2,1899)	1:76:A:ILE:HD11	1:73:A:SER:HB3	14	1.05
(2,1643)	1:91:A:ILE:HG21	1:93:A:ILE:H	6	1.05
(2,1556)	1:33:A:LYS:HB3	1:43:A:GLU:H	16	1.05
(2,1392)	1:119:A:ILE:HD13	1:116:A:THR:H	19	1.05
(2,761)	1:107:A:ASP:HB3	1:103:A:ILE:H	6	1.05
(2,118)	1:124:A:SER:HB3	1:123:A:LEU:H	17	1.05
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD11	14	1.04
(2,4300)	1:59:A:TYR:HB2	1:63:A:LEU:HD23	7	1.04
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD12	11	1.04
(2,4190)	1:64:A:VAL:HG23	1:24:A:ILE:HG21	11	1.04
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD12	1	1.04
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD11	8	1.04
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD12	20	1.04
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD13	17	1.04
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD13	15	1.04
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD13	2	1.04
(2,3905)	1:80:A:PHE:HE1	1:102:A:VAL:HG21	4	1.04
(2,3905)	1:80:A:PHE:HE1	1:102:A:VAL:HG22	8	1.04
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD23	3	1.04
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD11	16	1.04
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD13	6	1.04
(2,2377)	1:52:A:LEU:HD23	1:115:A:TYR:HA	4	1.04
(2,2377)	1:52:A:LEU:HD12	1:115:A:TYR:HA	6	1.04
(2,2373)	1:36:A:LEU:HD21	1:21:A:TYR:HA	12	1.04
(2,2338)	1:67:A:PRO:HG3	1:21:A:TYR:HA	1	1.04
(2,1885)	1:123:A:LEU:HD22	1:125:A:PRO:HA	14	1.04
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	13	1.04
(2,1643)	1:91:A:ILE:HG22	1:93:A:ILE:H	2	1.04
(2,1643)	1:94:A:LEU:HD23	1:93:A:ILE:H	12	1.04
(2,1643)	1:91:A:ILE:HG21	1:93:A:ILE:H	18	1.04
(2,1404)	1:69:A:ILE:HD12	1:37:A:ASN:HD22	3	1.04
(2,1402)	1:99:A:ILE:HG21	1:101:A:ASN:HD22	14	1.04
(2,1401)	1:106:A:VAL:HG21	1:105:A:ASN:HD22	17	1.04
(2,1392)	1:119:A:ILE:HD13	1:116:A:THR:H	14	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,168)	1:119:A:ILE:HG22	1:122:A:ILE:H	12	1.04
(2,4351)	1:111:A:LEU:HD23	1:91:A:ILE:HD12	12	1.03
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD11	3	1.03
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD12	15	1.03
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG21	3	1.03
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD11	10	1.03
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD13	15	1.03
(2,3243)	1:56:A:ILE:HD12	1:61:A:TRP:HB2	9	1.03
(2,2377)	1:52:A:LEU:HD11	1:115:A:TYR:HA	5	1.03
(2,2373)	1:36:A:LEU:HD21	1:21:A:TYR:HA	7	1.03
(2,2373)	1:36:A:LEU:HD22	1:21:A:TYR:HA	11	1.03
(2,2338)	1:65:A:LYS:HD3	1:21:A:TYR:HA	13	1.03
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	9	1.03
(2,1643)	1:91:A:ILE:HG22	1:93:A:ILE:H	5	1.03
(2,1643)	1:91:A:ILE:HG22	1:93:A:ILE:H	11	1.03
(2,1643)	1:91:A:ILE:HG23	1:93:A:ILE:H	17	1.03
(2,1643)	1:91:A:ILE:HG22	1:93:A:ILE:H	19	1.03
(2,1410)	1:119:A:ILE:HG21	1:116:A:THR:H	16	1.03
(2,1257)	1:108:A:VAL:HG12	1:113:A:ARG:H	14	1.03
(2,867)	1:99:A:ILE:HG21	1:88:A:LYS:H	12	1.03
(2,867)	1:99:A:ILE:HG21	1:88:A:LYS:H	13	1.03
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD12	11	1.02
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD11	9	1.02
(2,4122)	1:22:A:VAL:HA	1:66:A:ILE:HD12	5	1.02
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD12	14	1.02
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD13	20	1.02
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG23	18	1.02
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB2	17	1.02
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG11	20	1.02
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD21	6	1.02
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD13	3	1.02
(2,2873)	1:91:A:ILE:HD11	1:87:A:ASN:HB2	9	1.02
(2,2377)	1:52:A:LEU:HD12	1:115:A:TYR:HA	13	1.02
(2,2373)	1:36:A:LEU:HD23	1:21:A:TYR:HA	14	1.02
(2,2338)	1:65:A:LYS:HD3	1:21:A:TYR:HA	3	1.02
(2,1643)	1:91:A:ILE:HG21	1:93:A:ILE:H	8	1.02
(2,1497)	1:81:A:VAL:HG11	1:83:A:GLY:H	20	1.02
(2,1402)	1:99:A:ILE:HG23	1:101:A:ASN:HD22	9	1.02
(2,867)	1:64:A:VAL:HG12	1:88:A:LYS:H	9	1.02
(2,168)	1:119:A:ILE:HG22	1:122:A:ILE:H	11	1.02
(2,4384)	1:34:A:ILE:HG21	1:33:A:LYS:HB3	2	1.01
(2,4384)	1:34:A:ILE:HG22	1:33:A:LYS:HB3	15	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4384)	1:34:A:ILE:HG21	1:33:A:LYS:HB3	18	1.01
(2,4190)	1:64:A:VAL:HG21	1:24:A:ILE:HG21	12	1.01
(2,4071)	1:95:A:LEU:H	1:93:A:ILE:HD13	8	1.01
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG23	2	1.01
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG12	10	1.01
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD23	16	1.01
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD22	18	1.01
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG22	20	1.01
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD11	5	1.01
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD11	7	1.01
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD12	8	1.01
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD12	4	1.01
(2,2873)	1:91:A:ILE:HD12	1:87:A:ASN:HB2	8	1.01
(2,2873)	1:91:A:ILE:HD11	1:87:A:ASN:HB2	10	1.01
(2,2652)	1:95:A:LEU:HD21	1:107:A:ASP:HB2	15	1.01
(2,1643)	1:91:A:ILE:HG22	1:93:A:ILE:H	7	1.01
(2,1643)	1:94:A:LEU:HD21	1:93:A:ILE:H	20	1.01
(2,1404)	1:35:A:ARG:HG2	1:37:A:ASN:HD22	10	1.01
(2,1402)	1:99:A:ILE:HG22	1:101:A:ASN:HD22	10	1.01
(2,1392)	1:119:A:ILE:HD12	1:116:A:THR:H	17	1.01
(2,1257)	1:108:A:VAL:HG11	1:113:A:ARG:H	17	1.01
(2,1051)	1:106:A:VAL:HG21	1:109:A:GLU:H	10	1.01
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	10	1.01
(2,600)	1:91:A:ILE:HD13	1:69:A:ILE:H	16	1.01
(2,344)	1:108:A:VAL:HG13	1:71:A:ILE:H	20	1.01
(2,168)	1:119:A:ILE:HG22	1:122:A:ILE:H	7	1.01
(2,4300)	1:59:A:TYR:HB2	1:63:A:LEU:HD21	8	1.0
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD23	11	1.0
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD12	19	1.0
(2,4178)	1:28:A:LEU:HB3	1:24:A:ILE:HG22	8	1.0
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD12	4	1.0
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD13	9	1.0
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD11	8	1.0
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD21	6	1.0
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD21	9	1.0
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD12	13	1.0
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD12	18	1.0
(2,3243)	1:56:A:ILE:HD12	1:61:A:TRP:HB2	15	1.0
(2,2873)	1:91:A:ILE:HD13	1:87:A:ASN:HB2	16	1.0
(2,2373)	1:66:A:ILE:HD13	1:21:A:TYR:HA	10	1.0
(2,1556)	1:44:A:ILE:HB	1:43:A:GLU:H	12	1.0
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	17	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1497)	1:81:A:VAL:HG13	1:83:A:GLY:H	19	1.0
(2,1412)	1:119:A:ILE:HG23	1:114:A:GLU:H	11	1.0
(2,1402)	1:99:A:ILE:HG23	1:101:A:ASN:HD22	5	1.0
(2,889)	1:91:A:ILE:HD12	1:87:A:ASN:H	3	1.0
(2,867)	1:64:A:VAL:HG13	1:88:A:LYS:H	5	1.0
(2,316)	1:26:A:ASP:HB3	1:32:A:LEU:H	11	1.0
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD13	10	0.99
(2,3857)	1:24:A:ILE:HG22	1:49:A:VAL:HG21	12	0.99
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD22	16	0.99
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD23	15	0.99
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD23	16	0.99
(2,3689)	1:94:A:LEU:H	1:111:A:LEU:HD23	20	0.99
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG21	12	0.99
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG22	18	0.99
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD11	9	0.99
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD12	15	0.99
(2,2373)	1:36:A:LEU:HD21	1:21:A:TYR:HA	19	0.99
(2,1885)	1:122:A:ILE:HG22	1:125:A:PRO:HA	20	0.99
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	4	0.99
(2,1652)	1:112:A:LEU:HD11	1:110:A:LYS:H	16	0.99
(2,1556)	1:44:A:ILE:HB	1:43:A:GLU:H	2	0.99
(2,1556)	1:44:A:ILE:HB	1:43:A:GLU:H	3	0.99
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	4	0.99
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	18	0.99
(2,1497)	1:81:A:VAL:HG11	1:83:A:GLY:H	7	0.99
(2,1392)	1:119:A:ILE:HD12	1:116:A:THR:H	8	0.99
(2,761)	1:107:A:ASP:HB3	1:103:A:ILE:H	19	0.99
(2,168)	1:119:A:ILE:HG23	1:122:A:ILE:H	1	0.99
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD12	14	0.98
(2,4190)	1:64:A:VAL:HG23	1:24:A:ILE:HG23	10	0.98
(2,4190)	1:64:A:VAL:HG22	1:24:A:ILE:HG23	20	0.98
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD11	11	0.98
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD12	16	0.98
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD12	16	0.98
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG21	9	0.98
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG12	8	0.98
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD22	14	0.98
(2,3705)	1:14:A:PHE:HD1	1:10:A:LEU:HD23	8	0.98
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD11	2	0.98
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD12	20	0.98
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD13	18	0.98
(2,3111)	1:22:A:VAL:HA	1:65:A:LYS:HD3	19	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	14	0.98
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	15	0.98
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	6	0.98
(2,1404)	1:35:A:ARG:HG2	1:37:A:ASN:HD22	2	0.98
(2,1404)	1:122:A:ILE:HD11	1:37:A:ASN:HD22	17	0.98
(2,867)	1:99:A:ILE:HG21	1:88:A:LYS:H	20	0.98
(2,600)	1:91:A:ILE:HD11	1:69:A:ILE:H	17	0.98
(2,600)	1:91:A:ILE:HD12	1:69:A:ILE:H	20	0.98
(2,168)	1:119:A:ILE:HG21	1:122:A:ILE:H	8	0.98
(2,4209)	1:68:A:PHE:HA	1:91:A:ILE:HD13	1	0.97
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD13	6	0.97
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD11	17	0.97
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD12	3	0.97
(2,4093)	1:120:A:PHE:HD1	1:69:A:ILE:HD12	10	0.97
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG21	7	0.97
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG23	9	0.97
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD23	5	0.97
(2,3788)	1:91:A:ILE:HA	1:94:A:LEU:HD22	19	0.97
(2,3689)	1:94:A:LEU:H	1:111:A:LEU:HD23	10	0.97
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD23	19	0.97
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG23	10	0.97
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG21	19	0.97
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD13	5	0.97
(2,2873)	1:91:A:ILE:HD12	1:87:A:ASN:HB2	19	0.97
(2,1643)	1:91:A:ILE:HG21	1:93:A:ILE:H	15	0.97
(2,1392)	1:119:A:ILE:HD12	1:116:A:THR:H	16	0.97
(2,1389)	1:106:A:VAL:HG12	1:105:A:ASN:HD21	8	0.97
(2,1075)	1:119:A:ILE:HG22	1:115:A:TYR:H	13	0.97
(2,1059)	1:91:A:ILE:HG21	1:91:A:ILE:H	7	0.97
(2,1059)	1:91:A:ILE:HG23	1:91:A:ILE:H	15	0.97
(2,867)	1:64:A:VAL:HG11	1:88:A:LYS:H	4	0.97
(2,867)	1:99:A:ILE:HG23	1:88:A:LYS:H	15	0.97
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD21	6	0.96
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD12	17	0.96
(2,4190)	1:64:A:VAL:HG23	1:24:A:ILE:HG22	6	0.96
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD12	16	0.96
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD12	3	0.96
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD13	14	0.96
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD13	18	0.96
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD13	14	0.96
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD11	9	0.96
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD11	16	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3857)	1:24:A:ILE:HG21	1:49:A:VAL:HG22	17	0.96
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG21	9	0.96
(2,3271)	1:28:A:LEU:HD11	1:25:A:LYS:HD2	1	0.96
(2,2873)	1:91:A:ILE:HD13	1:87:A:ASN:HB2	12	0.96
(2,1885)	1:123:A:LEU:HD21	1:125:A:PRO:HA	8	0.96
(2,1643)	1:91:A:ILE:HG22	1:93:A:ILE:H	10	0.96
(2,1497)	1:81:A:VAL:HG13	1:83:A:GLY:H	10	0.96
(2,1059)	1:91:A:ILE:HG22	1:91:A:ILE:H	3	0.96
(2,1059)	1:91:A:ILE:HG21	1:91:A:ILE:H	5	0.96
(2,1059)	1:91:A:ILE:HG23	1:91:A:ILE:H	6	0.96
(2,1059)	1:91:A:ILE:HG21	1:91:A:ILE:H	8	0.96
(2,1059)	1:91:A:ILE:HG22	1:91:A:ILE:H	11	0.96
(2,1059)	1:91:A:ILE:HG21	1:91:A:ILE:H	12	0.96
(2,1059)	1:91:A:ILE:HG23	1:91:A:ILE:H	16	0.96
(2,1059)	1:91:A:ILE:HG23	1:91:A:ILE:H	17	0.96
(2,1059)	1:91:A:ILE:HG21	1:91:A:ILE:H	19	0.96
(2,168)	1:119:A:ILE:HG21	1:122:A:ILE:H	5	0.96
(2,4300)	1:65:A:LYS:HE2	1:63:A:LEU:HD22	3	0.95
(2,4190)	1:64:A:VAL:HG21	1:24:A:ILE:HG21	9	0.95
(2,4190)	1:64:A:VAL:HG22	1:24:A:ILE:HG21	16	0.95
(2,4190)	1:64:A:VAL:HG21	1:24:A:ILE:HG22	19	0.95
(2,4131)	1:60:A:LEU:HA	1:24:A:ILE:HD13	8	0.95
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD13	4	0.95
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD11	5	0.95
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD12	6	0.95
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD23	5	0.95
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG23	8	0.95
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG23	11	0.95
(2,3353)	1:24:A:ILE:H	1:25:A:LYS:HG2	6	0.95
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD11	17	0.95
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD12	20	0.95
(2,3243)	1:56:A:ILE:HD12	1:61:A:TRP:HB2	20	0.95
(2,2873)	1:91:A:ILE:HD13	1:87:A:ASN:HB2	7	0.95
(2,2873)	1:91:A:ILE:HD13	1:87:A:ASN:HB2	15	0.95
(2,2873)	1:91:A:ILE:HD11	1:87:A:ASN:HB2	18	0.95
(2,2652)	1:95:A:LEU:HD23	1:107:A:ASP:HB2	8	0.95
(2,2377)	1:52:A:LEU:HD11	1:115:A:TYR:HA	3	0.95
(2,2377)	1:52:A:LEU:HD13	1:115:A:TYR:HA	17	0.95
(2,2373)	1:36:A:LEU:HD23	1:21:A:TYR:HA	5	0.95
(2,1497)	1:81:A:VAL:HG13	1:83:A:GLY:H	9	0.95
(2,1402)	1:99:A:ILE:HG21	1:101:A:ASN:HD22	7	0.95
(2,1402)	1:99:A:ILE:HG21	1:101:A:ASN:HD22	11	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1257)	1:108:A:VAL:HG13	1:113:A:ARG:H	1	0.95
(2,1257)	1:108:A:VAL:HG12	1:113:A:ARG:H	12	0.95
(2,1066)	1:99:A:ILE:HD11	1:97:A:ARG:H	6	0.95
(2,1059)	1:91:A:ILE:HG22	1:91:A:ILE:H	1	0.95
(2,1059)	1:91:A:ILE:HG23	1:91:A:ILE:H	13	0.95
(2,867)	1:64:A:VAL:HG12	1:88:A:LYS:H	1	0.95
(2,607)	1:66:A:ILE:HG22	1:64:A:VAL:H	15	0.95
(2,316)	1:26:A:ASP:HB3	1:32:A:LEU:H	19	0.95
(2,168)	1:119:A:ILE:HG23	1:122:A:ILE:H	13	0.95
(2,4518)	1:76:A:ILE:HD13	1:80:A:PHE:HZ	18	0.94
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD11	2	0.94
(2,4243)	1:102:A:VAL:HG23	1:104:A:LEU:HA	12	0.94
(2,4209)	1:68:A:PHE:HA	1:91:A:ILE:HD12	5	0.94
(2,4209)	1:68:A:PHE:HA	1:91:A:ILE:HD11	10	0.94
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD13	11	0.94
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD12	7	0.94
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD11	2	0.94
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD13	2	0.94
(2,4084)	1:86:A:TRP:HE3	1:93:A:ILE:HD11	8	0.94
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG12	17	0.94
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD22	9	0.94
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD21	17	0.94
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG23	6	0.94
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG23	13	0.94
(2,3353)	1:24:A:ILE:H	1:25:A:LYS:HG3	3	0.94
(2,3243)	1:56:A:ILE:HD13	1:61:A:TRP:HB2	7	0.94
(2,2873)	1:91:A:ILE:HD12	1:87:A:ASN:HB2	11	0.94
(2,1404)	1:122:A:ILE:HD13	1:37:A:ASN:HD22	4	0.94
(2,1059)	1:91:A:ILE:HG21	1:91:A:ILE:H	20	0.94
(2,867)	1:99:A:ILE:HG22	1:88:A:LYS:H	3	0.94
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	1	0.94
(2,600)	1:91:A:ILE:HD12	1:69:A:ILE:H	14	0.94
(2,600)	1:91:A:ILE:HD11	1:69:A:ILE:H	18	0.94
(2,344)	1:108:A:VAL:HG12	1:71:A:ILE:H	3	0.94
(2,316)	1:26:A:ASP:HB3	1:32:A:LEU:H	6	0.94
(2,168)	1:119:A:ILE:HG22	1:122:A:ILE:H	10	0.94
(2,168)	1:119:A:ILE:HG23	1:122:A:ILE:H	19	0.94
(2,4244)	1:81:A:VAL:HG11	1:80:A:PHE:HA	13	0.93
(2,4190)	1:64:A:VAL:HG21	1:24:A:ILE:HG21	3	0.93
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG23	7	0.93
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD12	7	0.93
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD11	11	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG21	20	0.93
(2,3905)	1:80:A:PHE:HE1	1:102:A:VAL:HG22	15	0.93
(2,3857)	1:24:A:ILE:HG22	1:49:A:VAL:HG22	3	0.93
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG13	7	0.93
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD22	6	0.93
(2,3353)	1:24:A:ILE:H	1:25:A:LYS:HG2	17	0.93
(2,2377)	1:52:A:LEU:HD13	1:115:A:TYR:HA	19	0.93
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	8	0.93
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	14	0.93
(2,1643)	1:91:A:ILE:HG22	1:93:A:ILE:H	3	0.93
(2,1402)	1:99:A:ILE:HG23	1:101:A:ASN:HD22	20	0.93
(2,1059)	1:91:A:ILE:HG23	1:91:A:ILE:H	4	0.93
(2,1059)	1:91:A:ILE:HG22	1:91:A:ILE:H	10	0.93
(2,1059)	1:91:A:ILE:HG22	1:91:A:ILE:H	14	0.93
(2,1051)	1:106:A:VAL:HG22	1:109:A:GLU:H	17	0.93
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	4	0.93
(2,600)	1:91:A:ILE:HD12	1:69:A:ILE:H	13	0.93
(2,560)	1:95:A:LEU:HD11	1:104:A:LEU:H	16	0.93
(2,344)	1:108:A:VAL:HG13	1:71:A:ILE:H	11	0.93
(2,168)	1:119:A:ILE:HG23	1:122:A:ILE:H	16	0.93
(2,4394)	1:71:A:ILE:HG22	1:80:A:PHE:HB3	17	0.92
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD11	14	0.92
(2,4302)	1:89:A:LYS:HB3	1:63:A:LEU:HD11	19	0.92
(2,4244)	1:81:A:VAL:HG11	1:80:A:PHE:HA	2	0.92
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD11	2	0.92
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG21	3	0.92
(2,3857)	1:66:A:ILE:HG23	1:49:A:VAL:HG21	1	0.92
(2,3857)	1:66:A:ILE:HG22	1:49:A:VAL:HG21	18	0.92
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG23	5	0.92
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG22	16	0.92
(2,2873)	1:91:A:ILE:HD12	1:87:A:ASN:HB2	14	0.92
(2,2651)	1:95:A:LEU:HD23	1:110:A:LYS:HE3	8	0.92
(2,2373)	1:66:A:ILE:HD12	1:21:A:TYR:HA	9	0.92
(2,2194)	1:58:A:LEU:HD21	1:54:A:SER:HA	11	0.92
(2,1643)	1:91:A:ILE:HG23	1:93:A:ILE:H	4	0.92
(2,1643)	1:91:A:ILE:HG21	1:93:A:ILE:H	16	0.92
(2,1610)	1:95:A:LEU:HD23	1:110:A:LYS:H	12	0.92
(2,1412)	1:119:A:ILE:HG21	1:114:A:GLU:H	14	0.92
(2,1398)	1:111:A:LEU:HD21	1:114:A:GLU:H	5	0.92
(2,1059)	1:91:A:ILE:HG21	1:91:A:ILE:H	18	0.92
(2,600)	1:91:A:ILE:HD12	1:69:A:ILE:H	3	0.92
(2,600)	1:91:A:ILE:HD13	1:69:A:ILE:H	4	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,168)	1:119:A:ILE:HG21	1:122:A:ILE:H	4	0.92
(2,4351)	1:111:A:LEU:HD21	1:91:A:ILE:HD12	1	0.91
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD23	1	0.91
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD21	3	0.91
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD22	4	0.91
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD22	20	0.91
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD13	20	0.91
(2,4136)	1:5:A:ILE:HA	1:5:A:ILE:HD11	2	0.91
(2,4105)	1:79:A:TYR:HD1	1:71:A:ILE:HD11	2	0.91
(2,4105)	1:79:A:TYR:HD1	1:71:A:ILE:HD12	4	0.91
(2,4105)	1:79:A:TYR:HD1	1:71:A:ILE:HD13	9	0.91
(2,3857)	1:24:A:ILE:HG21	1:49:A:VAL:HG23	4	0.91
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD22	8	0.91
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD23	16	0.91
(2,2373)	1:36:A:LEU:HD23	1:21:A:TYR:HA	1	0.91
(2,2156)	1:121:A:ILE:HD12	1:121:A:ILE:HA	14	0.91
(2,1894)	1:5:A:ILE:HD11	1:5:A:ILE:HA	2	0.91
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	19	0.91
(2,1638)	1:24:A:ILE:HG22	1:62:A:SER:H	19	0.91
(2,1486)	1:69:A:ILE:HG13	1:83:A:GLY:H	2	0.91
(2,1402)	1:99:A:ILE:HG23	1:101:A:ASN:HD22	17	0.91
(2,1257)	1:108:A:VAL:HG12	1:113:A:ARG:H	16	0.91
(2,1257)	1:108:A:VAL:HG13	1:113:A:ARG:H	18	0.91
(2,1059)	1:91:A:ILE:HG22	1:91:A:ILE:H	2	0.91
(2,1059)	1:91:A:ILE:HG21	1:91:A:ILE:H	9	0.91
(2,867)	1:99:A:ILE:HG22	1:88:A:LYS:H	14	0.91
(2,168)	1:119:A:ILE:HG23	1:122:A:ILE:H	6	0.91
(2,168)	1:119:A:ILE:HG23	1:122:A:ILE:H	17	0.91
(2,116)	1:82:A:SER:HB3	1:120:A:PHE:H	13	0.91
(2,4518)	1:76:A:ILE:HD13	1:80:A:PHE:HZ	20	0.9
(2,4438)	1:35:A:ARG:HD3	1:41:A:TYR:HD1	10	0.9
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD23	9	0.9
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD23	12	0.9
(2,4244)	1:81:A:VAL:HG13	1:80:A:PHE:HA	4	0.9
(2,4244)	1:81:A:VAL:HG13	1:80:A:PHE:HA	11	0.9
(2,4244)	1:81:A:VAL:HG12	1:80:A:PHE:HA	19	0.9
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD13	12	0.9
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG21	13	0.9
(2,4161)	1:89:A:LYS:HE2	1:93:A:ILE:HD11	1	0.9
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD13	7	0.9
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD12	7	0.9
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG21	17	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG23	16	0.9
(2,3857)	1:66:A:ILE:HG22	1:49:A:VAL:HG21	20	0.9
(2,3788)	1:53:A:SER:HA	1:94:A:LEU:HD23	7	0.9
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD23	3	0.9
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD22	3	0.9
(2,3635)	1:52:A:LEU:HD12	1:56:A:ILE:HG12	19	0.9
(2,3520)	1:57:A:PRO:HD2	1:64:A:VAL:HG22	15	0.9
(2,3491)	1:95:A:LEU:HA	1:94:A:LEU:HD13	19	0.9
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD13	8	0.9
(2,3271)	1:28:A:LEU:HD13	1:25:A:LYS:HD2	12	0.9
(2,2156)	1:121:A:ILE:HD11	1:121:A:ILE:HA	1	0.9
(2,2156)	1:121:A:ILE:HD12	1:121:A:ILE:HA	3	0.9
(2,2156)	1:121:A:ILE:HD12	1:121:A:ILE:HA	4	0.9
(2,2156)	1:121:A:ILE:HD11	1:121:A:ILE:HA	5	0.9
(2,2156)	1:121:A:ILE:HD12	1:121:A:ILE:HA	12	0.9
(2,2156)	1:121:A:ILE:HD13	1:121:A:ILE:HA	20	0.9
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	10	0.9
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	20	0.9
(2,1404)	1:122:A:ILE:HD11	1:37:A:ASN:HD22	5	0.9
(2,1402)	1:99:A:ILE:HG22	1:101:A:ASN:HD22	18	0.9
(2,1402)	1:99:A:ILE:HG21	1:101:A:ASN:HD22	19	0.9
(2,1399)	1:56:A:ILE:HG21	1:55:A:ARG:HE	8	0.9
(2,1257)	1:108:A:VAL:HG11	1:113:A:ARG:H	3	0.9
(2,1257)	1:108:A:VAL:HG12	1:113:A:ARG:H	11	0.9
(2,1051)	1:106:A:VAL:HG22	1:109:A:GLU:H	16	0.9
(2,1051)	1:106:A:VAL:HG22	1:109:A:GLU:H	20	0.9
(2,867)	1:64:A:VAL:HG12	1:88:A:LYS:H	17	0.9
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	7	0.9
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	8	0.9
(2,344)	1:108:A:VAL:HG11	1:71:A:ILE:H	7	0.9
(2,344)	1:108:A:VAL:HG11	1:71:A:ILE:H	18	0.9
(2,4518)	1:76:A:ILE:HD11	1:80:A:PHE:HZ	14	0.89
(2,4394)	1:71:A:ILE:HG22	1:80:A:PHE:HB3	10	0.89
(2,4384)	1:34:A:ILE:HG21	1:33:A:LYS:HB3	6	0.89
(2,4351)	1:111:A:LEU:HD23	1:91:A:ILE:HD11	11	0.89
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD11	20	0.89
(2,4244)	1:81:A:VAL:HG12	1:80:A:PHE:HA	9	0.89
(2,4244)	1:81:A:VAL:HG12	1:80:A:PHE:HA	17	0.89
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD11	17	0.89
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG21	11	0.89
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD12	14	0.89
(2,4131)	1:60:A:LEU:HA	1:24:A:ILE:HD12	7	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD11	20	0.89
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG22	13	0.89
(2,3857)	1:66:A:ILE:HG22	1:49:A:VAL:HG21	14	0.89
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD23	4	0.89
(2,3708)	1:64:A:VAL:H	1:64:A:VAL:HG13	8	0.89
(2,3689)	1:94:A:LEU:H	1:111:A:LEU:HD23	4	0.89
(2,3681)	1:74:A:SER:H	1:126:A:THR:HG23	1	0.89
(2,3353)	1:24:A:ILE:H	1:25:A:LYS:HG3	4	0.89
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	1	0.89
(2,2373)	1:66:A:ILE:HD13	1:21:A:TYR:HA	4	0.89
(2,2373)	1:36:A:LEU:HD22	1:21:A:TYR:HA	8	0.89
(2,2156)	1:121:A:ILE:HD13	1:121:A:ILE:HA	10	0.89
(2,2156)	1:121:A:ILE:HD12	1:121:A:ILE:HA	13	0.89
(2,1666)	1:121:A:ILE:HD12	1:121:A:ILE:H	5	0.89
(2,1486)	1:69:A:ILE:HG13	1:83:A:GLY:H	5	0.89
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	15	0.89
(2,1401)	1:106:A:VAL:HG21	1:105:A:ASN:HD22	18	0.89
(2,1398)	1:119:A:ILE:HD13	1:114:A:GLU:H	18	0.89
(2,1392)	1:119:A:ILE:HD12	1:116:A:THR:H	13	0.89
(2,1257)	1:108:A:VAL:HG12	1:113:A:ARG:H	20	0.89
(2,344)	1:108:A:VAL:HG13	1:71:A:ILE:H	2	0.89
(2,235)	1:31:A:LYS:HB3	1:27:A:ALA:H	8	0.89
(2,168)	1:119:A:ILE:HG22	1:122:A:ILE:H	3	0.89
(2,4518)	1:102:A:VAL:HG21	1:80:A:PHE:HZ	17	0.88
(2,4394)	1:71:A:ILE:HG21	1:80:A:PHE:HB3	9	0.88
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB1	20	0.88
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD11	18	0.88
(2,4190)	1:64:A:VAL:HG23	1:24:A:ILE:HG21	1	0.88
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG23	20	0.88
(2,4105)	1:59:A:TYR:HE2	1:93:A:ILE:HD11	5	0.88
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD11	6	0.88
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD12	4	0.88
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD11	5	0.88
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD11	13	0.88
(2,3966)	1:98:A:GLU:HA	1:99:A:ILE:HG23	17	0.88
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG23	1	0.88
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB3	19	0.88
(2,3857)	1:66:A:ILE:HG23	1:49:A:VAL:HG23	7	0.88
(2,3708)	1:64:A:VAL:H	1:64:A:VAL:HG13	7	0.88
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD21	5	0.88
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD22	11	0.88
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD23	14	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3681)	1:75:A:GLU:H	1:126:A:THR:HG21	9	0.88
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD11	10	0.88
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD11	19	0.88
(2,2865)	1:104:A:LEU:HD23	1:105:A:ASN:HB3	13	0.88
(2,2156)	1:122:A:ILE:HD13	1:121:A:ILE:HA	7	0.88
(2,2156)	1:121:A:ILE:HD13	1:121:A:ILE:HA	18	0.88
(2,2156)	1:121:A:ILE:HD13	1:121:A:ILE:HA	19	0.88
(2,1643)	1:91:A:ILE:HG22	1:93:A:ILE:H	14	0.88
(2,1610)	1:95:A:LEU:HD22	1:110:A:LYS:H	17	0.88
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	15	0.88
(2,1497)	1:81:A:VAL:HG11	1:83:A:GLY:H	16	0.88
(2,1399)	1:93:A:ILE:HG23	1:55:A:ARG:HE	2	0.88
(2,600)	1:91:A:ILE:HD11	1:69:A:ILE:H	9	0.88
(2,344)	1:108:A:VAL:HG13	1:71:A:ILE:H	12	0.88
(2,235)	1:25:A:LYS:HB3	1:27:A:ALA:H	19	0.88
(2,4518)	1:76:A:ILE:HD12	1:80:A:PHE:HZ	3	0.87
(2,4414)	1:137:A:GLU:HG2	1:133:A:THR:HB	7	0.87
(2,4394)	1:71:A:ILE:HG23	1:80:A:PHE:HB3	16	0.87
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD22	15	0.87
(2,4244)	1:81:A:VAL:HG11	1:80:A:PHE:HA	5	0.87
(2,4244)	1:81:A:VAL:HG12	1:80:A:PHE:HA	6	0.87
(2,4244)	1:81:A:VAL:HG13	1:80:A:PHE:HA	7	0.87
(2,4244)	1:81:A:VAL:HG13	1:80:A:PHE:HA	12	0.87
(2,4244)	1:81:A:VAL:HG13	1:80:A:PHE:HA	15	0.87
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD13	1	0.87
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD13	16	0.87
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG21	9	0.87
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD13	6	0.87
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD12	1	0.87
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD12	20	0.87
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD11	16	0.87
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD11	19	0.87
(2,4093)	1:120:A:PHE:HD1	1:122:A:ILE:HD11	6	0.87
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD13	6	0.87
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG22	10	0.87
(2,3966)	1:98:A:GLU:HA	1:99:A:ILE:HG22	10	0.87
(2,3857)	1:66:A:ILE:HG22	1:49:A:VAL:HG22	10	0.87
(2,3857)	1:66:A:ILE:HG21	1:49:A:VAL:HG22	11	0.87
(2,3857)	1:66:A:ILE:HG21	1:49:A:VAL:HG21	16	0.87
(2,3708)	1:64:A:VAL:H	1:64:A:VAL:HG11	3	0.87
(2,3708)	1:64:A:VAL:H	1:64:A:VAL:HG12	12	0.87
(2,3111)	1:22:A:VAL:HA	1:65:A:LYS:HD3	3	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2873)	1:91:A:ILE:HD13	1:87:A:ASN:HB2	4	0.87
(2,2873)	1:91:A:ILE:HD12	1:87:A:ASN:HB2	6	0.87
(2,2652)	1:95:A:LEU:HD23	1:107:A:ASP:HB2	3	0.87
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	3	0.87
(2,2382)	1:103:A:ILE:HG13	1:107:A:ASP:HA	18	0.87
(2,2163)	1:102:A:VAL:HG22	1:103:A:ILE:HA	16	0.87
(2,2156)	1:121:A:ILE:HD12	1:121:A:ILE:HA	16	0.87
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	11	0.87
(2,1666)	1:122:A:ILE:HD12	1:121:A:ILE:H	11	0.87
(2,1666)	1:121:A:ILE:HD13	1:121:A:ILE:H	12	0.87
(2,1610)	1:95:A:LEU:HD23	1:110:A:LYS:H	6	0.87
(2,1497)	1:81:A:VAL:HG12	1:83:A:GLY:H	1	0.87
(2,1404)	1:69:A:ILE:HD13	1:37:A:ASN:HD22	12	0.87
(2,1051)	1:106:A:VAL:HG23	1:109:A:GLU:H	1	0.87
(2,1051)	1:106:A:VAL:HG23	1:109:A:GLU:H	19	0.87
(2,867)	1:99:A:ILE:HG22	1:88:A:LYS:H	7	0.87
(2,867)	1:99:A:ILE:HG23	1:88:A:LYS:H	18	0.87
(2,761)	1:107:A:ASP:HB3	1:103:A:ILE:H	3	0.87
(2,665)	1:115:A:TYR:HE2	1:112:A:LEU:H	7	0.87
(2,600)	1:91:A:ILE:HD12	1:69:A:ILE:H	11	0.87
(2,600)	1:91:A:ILE:HD12	1:69:A:ILE:H	19	0.87
(2,4518)	1:76:A:ILE:HD11	1:80:A:PHE:HZ	1	0.86
(2,4394)	1:71:A:ILE:HG22	1:80:A:PHE:HB3	11	0.86
(2,4244)	1:81:A:VAL:HG11	1:80:A:PHE:HA	8	0.86
(2,4244)	1:81:A:VAL:HG12	1:80:A:PHE:HA	14	0.86
(2,4244)	1:81:A:VAL:HG13	1:80:A:PHE:HA	16	0.86
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD13	4	0.86
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD12	19	0.86
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG23	10	0.86
(2,4131)	1:60:A:LEU:HA	1:24:A:ILE:HD12	5	0.86
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD12	9	0.86
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD11	2	0.86
(2,3905)	1:80:A:PHE:HE1	1:102:A:VAL:HG22	11	0.86
(2,3708)	1:64:A:VAL:H	1:64:A:VAL:HG13	11	0.86
(2,3361)	1:60:A:LEU:H	1:64:A:VAL:HG22	2	0.86
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD13	12	0.86
(2,2651)	1:95:A:LEU:HD22	1:110:A:LYS:HE3	1	0.86
(2,2651)	1:95:A:LEU:HD22	1:110:A:LYS:HE3	6	0.86
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	18	0.86
(2,2375)	1:118:A:LEU:HD11	1:115:A:TYR:HA	12	0.86
(2,2373)	1:36:A:LEU:HD23	1:21:A:TYR:HA	16	0.86
(2,2156)	1:121:A:ILE:HD12	1:121:A:ILE:HA	2	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2156)	1:121:A:ILE:HD13	1:121:A:ILE:HA	15	0.86
(2,1666)	1:121:A:ILE:HD13	1:121:A:ILE:H	7	0.86
(2,1666)	1:121:A:ILE:HD11	1:121:A:ILE:H	20	0.86
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	13	0.86
(2,1497)	1:81:A:VAL:HG11	1:83:A:GLY:H	4	0.86
(2,1402)	1:99:A:ILE:HG23	1:101:A:ASN:HD22	13	0.86
(2,1389)	1:106:A:VAL:HG11	1:105:A:ASN:HD21	9	0.86
(2,1051)	1:106:A:VAL:HG21	1:109:A:GLU:H	2	0.86
(2,607)	1:66:A:ILE:HG21	1:64:A:VAL:H	6	0.86
(2,600)	1:91:A:ILE:HD13	1:69:A:ILE:H	1	0.86
(2,316)	1:31:A:LYS:HE2	1:32:A:LEU:H	4	0.86
(2,4394)	1:71:A:ILE:HG23	1:80:A:PHE:HB3	3	0.85
(2,4394)	1:71:A:ILE:HG21	1:80:A:PHE:HB3	12	0.85
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD23	16	0.85
(2,4244)	1:81:A:VAL:HG13	1:80:A:PHE:HA	20	0.85
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD13	1	0.85
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD12	20	0.85
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD12	2	0.85
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD13	7	0.85
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG21	1	0.85
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG21	16	0.85
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD11	16	0.85
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD11	13	0.85
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD11	12	0.85
(2,4122)	1:23:A:THR:HB	1:66:A:ILE:HD13	17	0.85
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD12	10	0.85
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD11	11	0.85
(2,3708)	1:64:A:VAL:H	1:64:A:VAL:HG11	14	0.85
(2,3708)	1:64:A:VAL:H	1:64:A:VAL:HG12	20	0.85
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD22	4	0.85
(2,3635)	1:52:A:LEU:HD11	1:56:A:ILE:HG12	6	0.85
(2,2373)	1:36:A:LEU:HD21	1:21:A:TYR:HA	6	0.85
(2,2194)	1:28:A:LEU:HD12	1:54:A:SER:HA	3	0.85
(2,2163)	1:102:A:VAL:HG23	1:103:A:ILE:HA	5	0.85
(2,2156)	1:121:A:ILE:HD12	1:121:A:ILE:HA	9	0.85
(2,2156)	1:121:A:ILE:HD13	1:121:A:ILE:HA	11	0.85
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	18	0.85
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	15	0.85
(2,1714)	1:131:A:GLU:HB2	1:130:A:THR:HB	13	0.85
(2,1409)	1:66:A:ILE:HG21	1:87:A:ASN:HD21	13	0.85
(2,1402)	1:99:A:ILE:HG22	1:101:A:ASN:HD22	2	0.85
(2,1402)	1:99:A:ILE:HG21	1:101:A:ASN:HD22	6	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1398)	1:111:A:LEU:HD21	1:114:A:GLU:H	2	0.85
(2,1398)	1:111:A:LEU:HD21	1:114:A:GLU:H	20	0.85
(2,600)	1:91:A:ILE:HD13	1:69:A:ILE:H	7	0.85
(2,560)	1:95:A:LEU:HD11	1:104:A:LEU:H	15	0.85
(2,316)	1:26:A:ASP:HB3	1:32:A:LEU:H	1	0.85
(2,4689)	1:72:A:LYS:HG2	1:79:A:TYR:HD2	6	0.84
(2,4394)	1:71:A:ILE:HG21	1:80:A:PHE:HB3	18	0.84
(2,4394)	1:71:A:ILE:HG21	1:80:A:PHE:HB3	19	0.84
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD21	17	0.84
(2,4244)	1:81:A:VAL:HG13	1:80:A:PHE:HA	3	0.84
(2,4244)	1:81:A:VAL:HG12	1:80:A:PHE:HA	10	0.84
(2,4244)	1:81:A:VAL:HG13	1:80:A:PHE:HA	18	0.84
(2,4243)	1:102:A:VAL:HG22	1:104:A:LEU:HA	4	0.84
(2,4243)	1:102:A:VAL:HG23	1:104:A:LEU:HA	15	0.84
(2,4131)	1:60:A:LEU:HA	1:24:A:ILE:HD11	12	0.84
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD13	8	0.84
(2,4107)	1:21:A:TYR:HD2	1:34:A:ILE:HD12	8	0.84
(2,4092)	1:14:A:PHE:HD2	1:122:A:ILE:HD11	13	0.84
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD13	8	0.84
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD13	12	0.84
(2,4026)	1:52:A:LEU:HB3	1:66:A:ILE:HG23	7	0.84
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD22	2	0.84
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD23	7	0.84
(2,3353)	1:24:A:ILE:H	1:25:A:LYS:HG3	18	0.84
(2,2652)	1:95:A:LEU:HD22	1:107:A:ASP:HB2	19	0.84
(2,2156)	1:122:A:ILE:HD13	1:121:A:ILE:HA	17	0.84
(2,1896)	1:94:A:LEU:HD13	1:93:A:ILE:HA	1	0.84
(2,1885)	1:123:A:LEU:HD22	1:125:A:PRO:HA	19	0.84
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	1	0.84
(2,1833)	1:51:A:LYS:HB2	1:54:A:SER:HB2	8	0.84
(2,1666)	1:121:A:ILE:HD13	1:121:A:ILE:H	13	0.84
(2,1486)	1:69:A:ILE:HG13	1:83:A:GLY:H	3	0.84
(2,1402)	1:99:A:ILE:HG23	1:101:A:ASN:HD22	4	0.84
(2,1389)	1:106:A:VAL:HG11	1:105:A:ASN:HD21	11	0.84
(2,1257)	1:108:A:VAL:HG12	1:113:A:ARG:H	6	0.84
(2,1257)	1:108:A:VAL:HG11	1:113:A:ARG:H	13	0.84
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	13	0.84
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	17	0.84
(2,344)	1:108:A:VAL:HG13	1:71:A:ILE:H	14	0.84
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	7	0.84
(2,235)	1:25:A:LYS:HB3	1:27:A:ALA:H	20	0.84
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD12	7	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4300)	1:65:A:LYS:HE3	1:63:A:LEU:HD22	5	0.83
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD21	13	0.83
(2,4244)	1:81:A:VAL:HG11	1:80:A:PHE:HA	1	0.83
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD12	11	0.83
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD12	14	0.83
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD11	18	0.83
(2,4190)	1:64:A:VAL:HG22	1:24:A:ILE:HG23	4	0.83
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD13	2	0.83
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD13	17	0.83
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD12	6	0.83
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD13	15	0.83
(2,3838)	1:31:A:LYS:HG2	1:22:A:VAL:HG12	6	0.83
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD23	18	0.83
(2,2652)	1:95:A:LEU:HD23	1:107:A:ASP:HB2	6	0.83
(2,2652)	1:95:A:LEU:HD21	1:107:A:ASP:HB2	16	0.83
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	6	0.83
(2,2156)	1:122:A:ILE:HD13	1:121:A:ILE:HA	8	0.83
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	6	0.83
(2,1666)	1:121:A:ILE:HD12	1:121:A:ILE:H	1	0.83
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	7	0.83
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	16	0.83
(2,1257)	1:108:A:VAL:HG12	1:113:A:ARG:H	2	0.83
(2,1257)	1:108:A:VAL:HG11	1:113:A:ARG:H	15	0.83
(2,1051)	1:106:A:VAL:HG21	1:109:A:GLU:H	5	0.83
(2,168)	1:119:A:ILE:HG21	1:122:A:ILE:H	15	0.83
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD1	3	0.82
(2,4394)	1:71:A:ILE:HG23	1:80:A:PHE:HB3	8	0.82
(2,4278)	1:91:A:ILE:H	1:52:A:LEU:HD13	20	0.82
(2,4190)	1:64:A:VAL:HG22	1:24:A:ILE:HG21	18	0.82
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD11	15	0.82
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD12	12	0.82
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD12	19	0.82
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD11	20	0.82
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG22	2	0.82
(2,3857)	1:66:A:ILE:HG21	1:49:A:VAL:HG22	5	0.82
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD23	8	0.82
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD22	6	0.82
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG23	19	0.82
(2,3353)	1:24:A:ILE:H	1:25:A:LYS:HG2	12	0.82
(2,3111)	1:21:A:TYR:HA	1:65:A:LYS:HD3	10	0.82
(2,2382)	1:28:A:LEU:HD23	1:47:A:ASP:HA	14	0.82
(2,2338)	1:65:A:LYS:HD3	1:21:A:TYR:HA	10	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	2	0.82
(2,1885)	1:122:A:ILE:HG21	1:125:A:PRO:HA	17	0.82
(2,1833)	1:50:A:GLU:HB3	1:54:A:SER:HB2	12	0.82
(2,1401)	1:106:A:VAL:HG22	1:105:A:ASN:HD22	3	0.82
(2,1398)	1:119:A:ILE:HD12	1:114:A:GLU:H	16	0.82
(2,1066)	1:99:A:ILE:HD13	1:97:A:ARG:H	16	0.82
(2,1051)	1:106:A:VAL:HG22	1:109:A:GLU:H	18	0.82
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	14	0.82
(2,560)	1:95:A:LEU:HD13	1:104:A:LEU:H	6	0.82
(2,235)	1:31:A:LYS:HB3	1:27:A:ALA:H	11	0.82
(2,4551)	1:122:A:ILE:HD12	1:120:A:PHE:HE2	9	0.81
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	17	0.81
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD1	15	0.81
(2,4438)	1:35:A:ARG:HD3	1:41:A:TYR:HD2	9	0.81
(2,4394)	1:71:A:ILE:HG21	1:80:A:PHE:HB3	2	0.81
(2,4394)	1:71:A:ILE:HG23	1:80:A:PHE:HB3	6	0.81
(2,4254)	1:46:A:LYS:HG2	1:47:A:ASP:HB3	14	0.81
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD11	10	0.81
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD12	5	0.81
(2,4190)	1:64:A:VAL:HG21	1:24:A:ILE:HG23	2	0.81
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG23	4	0.81
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD11	10	0.81
(2,4131)	1:60:A:LEU:HA	1:24:A:ILE:HD13	19	0.81
(2,4097)	1:68:A:PHE:HD2	1:66:A:ILE:HD11	13	0.81
(2,4093)	1:120:A:PHE:HD1	1:69:A:ILE:HD12	11	0.81
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD11	3	0.81
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD13	7	0.81
(2,3857)	1:66:A:ILE:HG21	1:49:A:VAL:HG22	2	0.81
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD22	15	0.81
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD22	8	0.81
(2,3689)	1:94:A:LEU:H	1:111:A:LEU:HD23	2	0.81
(2,3409)	1:59:A:TYR:HE1	1:60:A:LEU:HD21	8	0.81
(2,3353)	1:24:A:ILE:H	1:25:A:LYS:HG3	14	0.81
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	2	0.81
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	5	0.81
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	7	0.81
(2,2194)	1:28:A:LEU:HD12	1:54:A:SER:HA	19	0.81
(2,2174)	1:60:A:LEU:HG	1:59:A:TYR:HA	13	0.81
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	7	0.81
(2,1666)	1:121:A:ILE:HD13	1:121:A:ILE:H	2	0.81
(2,1666)	1:121:A:ILE:HD11	1:121:A:ILE:H	10	0.81
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	13	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1404)	1:122:A:ILE:HD12	1:37:A:ASN:HD22	1	0.81
(2,1402)	1:99:A:ILE:HG21	1:101:A:ASN:HD22	3	0.81
(2,1389)	1:106:A:VAL:HG21	1:105:A:ASN:HD21	20	0.81
(2,761)	1:107:A:ASP:HB3	1:103:A:ILE:H	5	0.81
(2,560)	1:95:A:LEU:HD11	1:104:A:LEU:H	5	0.81
(2,235)	1:31:A:LYS:HB3	1:27:A:ALA:H	9	0.81
(2,235)	1:31:A:LYS:HB3	1:27:A:ALA:H	15	0.81
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD2	11	0.8
(2,4351)	1:111:A:LEU:HD23	1:91:A:ILE:HD13	18	0.8
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG22	6	0.8
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD22	14	0.8
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG21	3	0.8
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG21	15	0.8
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD12	17	0.8
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD11	7	0.8
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD11	19	0.8
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG21	2	0.8
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG23	11	0.8
(2,3973)	1:81:A:VAL:HA	1:119:A:ILE:HG22	14	0.8
(2,3857)	1:66:A:ILE:HG22	1:49:A:VAL:HG21	13	0.8
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD22	14	0.8
(2,3681)	1:75:A:GLU:H	1:126:A:THR:HG22	5	0.8
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD21	13	0.8
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG23	9	0.8
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG22	17	0.8
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD12	9	0.8
(2,3271)	1:58:A:LEU:HD23	1:25:A:LYS:HD2	17	0.8
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	5	0.8
(2,2652)	1:95:A:LEU:HD22	1:107:A:ASP:HB2	5	0.8
(2,2194)	1:28:A:LEU:HD13	1:54:A:SER:HA	15	0.8
(2,2174)	1:60:A:LEU:HG	1:59:A:TYR:HA	2	0.8
(2,2163)	1:102:A:VAL:HG23	1:103:A:ILE:HA	12	0.8
(2,1896)	1:60:A:LEU:HD12	1:93:A:ILE:HA	18	0.8
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	5	0.8
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	17	0.8
(2,1666)	1:121:A:ILE:HD13	1:121:A:ILE:H	16	0.8
(2,1666)	1:121:A:ILE:HD11	1:121:A:ILE:H	18	0.8
(2,1550)	1:50:A:GLU:HG2	1:46:A:LYS:H	13	0.8
(2,1501)	1:95:A:LEU:HD12	1:96:A:GLY:H	18	0.8
(2,1497)	1:81:A:VAL:HG11	1:83:A:GLY:H	3	0.8
(2,1398)	1:119:A:ILE:HD13	1:114:A:GLU:H	19	0.8
(2,1389)	1:106:A:VAL:HG13	1:105:A:ASN:HD21	13	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1256)	1:28:A:LEU:HD12	1:54:A:SER:H	19	0.8
(2,1066)	1:99:A:ILE:HD13	1:97:A:ARG:H	1	0.8
(2,1051)	1:106:A:VAL:HG23	1:109:A:GLU:H	3	0.8
(2,1051)	1:106:A:VAL:HG21	1:109:A:GLU:H	6	0.8
(2,1051)	1:106:A:VAL:HG22	1:109:A:GLU:H	14	0.8
(2,867)	1:99:A:ILE:HG22	1:88:A:LYS:H	11	0.8
(2,600)	1:91:A:ILE:HD12	1:69:A:ILE:H	8	0.8
(2,316)	1:26:A:ASP:HB3	1:32:A:LEU:H	2	0.8
(2,235)	1:31:A:LYS:HB3	1:27:A:ALA:H	16	0.8
(2,4394)	1:71:A:ILE:HG22	1:80:A:PHE:HB3	20	0.79
(2,4351)	1:111:A:LEU:HD23	1:91:A:ILE:HD11	6	0.79
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD21	18	0.79
(2,4243)	1:102:A:VAL:HG22	1:104:A:LEU:HA	3	0.79
(2,4222)	1:75:A:GLU:HB3	1:73:A:SER:HB3	15	0.79
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD11	17	0.79
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG21	12	0.79
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG23	17	0.79
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD11	20	0.79
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD11	4	0.79
(2,4131)	1:60:A:LEU:HA	1:24:A:ILE:HD11	16	0.79
(2,4105)	1:59:A:TYR:HE1	1:93:A:ILE:HD12	8	0.79
(2,4097)	1:68:A:PHE:HD1	1:66:A:ILE:HD13	1	0.79
(2,4093)	1:120:A:PHE:HD1	1:122:A:ILE:HD11	12	0.79
(2,4093)	1:120:A:PHE:HD1	1:122:A:ILE:HD11	19	0.79
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG22	16	0.79
(2,3857)	1:66:A:ILE:HG23	1:49:A:VAL:HG23	19	0.79
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD21	8	0.79
(2,2874)	1:49:A:VAL:HG23	1:48:A:GLU:HG3	12	0.79
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	4	0.79
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	13	0.79
(2,2382)	1:103:A:ILE:HG13	1:107:A:ASP:HA	4	0.79
(2,1896)	1:60:A:LEU:HD13	1:93:A:ILE:HA	20	0.79
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	15	0.79
(2,1398)	1:119:A:ILE:HD13	1:114:A:GLU:H	7	0.79
(2,1398)	1:119:A:ILE:HD12	1:114:A:GLU:H	17	0.79
(2,1257)	1:108:A:VAL:HG13	1:113:A:ARG:H	7	0.79
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	6	0.79
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	11	0.79
(2,348)	1:24:A:ILE:HG22	1:61:A:TRP:H	19	0.79
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE2	6	0.78
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	14	0.78
(2,4394)	1:71:A:ILE:HG22	1:80:A:PHE:HB3	1	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4394)	1:71:A:ILE:HG23	1:80:A:PHE:HB3	5	0.78
(2,4394)	1:71:A:ILE:HG23	1:80:A:PHE:HB3	15	0.78
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB2	8	0.78
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD12	20	0.78
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG23	2	0.78
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD13	19	0.78
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD13	14	0.78
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD11	20	0.78
(2,4092)	1:14:A:PHE:HD1	1:122:A:ILE:HD11	17	0.78
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD12	10	0.78
(2,4006)	1:80:A:PHE:HB3	1:99:A:ILE:HG23	6	0.78
(2,3966)	1:98:A:GLU:HA	1:99:A:ILE:HG21	14	0.78
(2,3857)	1:66:A:ILE:HG23	1:49:A:VAL:HG23	6	0.78
(2,3857)	1:66:A:ILE:HG22	1:49:A:VAL:HG23	8	0.78
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG12	14	0.78
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD22	15	0.78
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD23	2	0.78
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG12	2	0.78
(2,3409)	1:79:A:TYR:HD1	1:123:A:LEU:HD21	2	0.78
(2,3353)	1:24:A:ILE:H	1:25:A:LYS:HG2	1	0.78
(2,2542)	1:115:A:TYR:HD1	1:111:A:LEU:HB2	13	0.78
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	8	0.78
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	17	0.78
(2,2373)	1:36:A:LEU:HD21	1:21:A:TYR:HA	2	0.78
(2,2163)	1:102:A:VAL:HG22	1:103:A:ILE:HA	10	0.78
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	4	0.78
(2,1666)	1:121:A:ILE:HD13	1:121:A:ILE:H	3	0.78
(2,1501)	1:95:A:LEU:HD11	1:96:A:GLY:H	7	0.78
(2,1402)	1:99:A:ILE:HG22	1:101:A:ASN:HD22	15	0.78
(2,1066)	1:99:A:ILE:HD11	1:97:A:ARG:H	7	0.78
(2,331)	1:33:A:LYS:HB3	1:32:A:LEU:H	14	0.78
(2,168)	1:119:A:ILE:HG22	1:122:A:ILE:H	18	0.78
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE1	16	0.77
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE2	16	0.77
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD13	10	0.77
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD22	5	0.77
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD23	10	0.77
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD11	18	0.77
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD12	19	0.77
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD12	8	0.77
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD12	13	0.77
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD12	17	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4105)	1:59:A:TYR:HE1	1:93:A:ILE:HD13	11	0.77
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD12	20	0.77
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD12	18	0.77
(2,4006)	1:80:A:PHE:HB3	1:99:A:ILE:HG21	15	0.77
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	17	0.77
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD23	8	0.77
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD22	12	0.77
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD22	13	0.77
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD21	20	0.77
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG21	6	0.77
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD21	12	0.77
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	16	0.77
(2,2382)	1:103:A:ILE:HG13	1:107:A:ASP:HA	10	0.77
(2,2174)	1:60:A:LEU:HG	1:59:A:TYR:HA	12	0.77
(2,2156)	1:122:A:ILE:HD11	1:121:A:ILE:HA	6	0.77
(2,1896)	1:60:A:LEU:HD13	1:93:A:ILE:HA	9	0.77
(2,1896)	1:60:A:LEU:HD11	1:93:A:ILE:HA	14	0.77
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	15	0.77
(2,1557)	1:24:A:ILE:HD12	1:61:A:TRP:HE1	3	0.77
(2,1557)	1:24:A:ILE:HD13	1:61:A:TRP:HE1	6	0.77
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	2	0.77
(2,1412)	1:119:A:ILE:HG22	1:114:A:GLU:H	13	0.77
(2,1404)	1:35:A:ARG:HG2	1:37:A:ASN:HD22	14	0.77
(2,1401)	1:106:A:VAL:HG22	1:105:A:ASN:HD22	19	0.77
(2,1398)	1:119:A:ILE:HD11	1:114:A:GLU:H	3	0.77
(2,1398)	1:119:A:ILE:HD12	1:114:A:GLU:H	12	0.77
(2,1066)	1:99:A:ILE:HD11	1:97:A:ARG:H	10	0.77
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	16	0.77
(2,610)	1:24:A:ILE:HG23	1:63:A:LEU:H	20	0.77
(2,596)	1:28:A:LEU:HD13	1:50:A:GLU:H	15	0.77
(2,560)	1:95:A:LEU:HD13	1:104:A:LEU:H	2	0.77
(2,560)	1:95:A:LEU:HD12	1:104:A:LEU:H	3	0.77
(2,560)	1:95:A:LEU:HD12	1:104:A:LEU:H	17	0.77
(2,316)	1:26:A:ASP:HB3	1:32:A:LEU:H	16	0.77
(2,316)	1:26:A:ASP:HB3	1:32:A:LEU:H	20	0.77
(2,118)	1:125:A:PRO:HD3	1:123:A:LEU:H	3	0.77
(2,116)	1:17:A:SER:HB3	1:120:A:PHE:H	7	0.77
(2,4518)	1:76:A:ILE:HD12	1:80:A:PHE:HZ	12	0.76
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD2	6	0.76
(2,4458)	1:20:A:GLU:HB2	1:21:A:TYR:HD2	10	0.76
(2,4394)	1:71:A:ILE:HG21	1:80:A:PHE:HB3	4	0.76
(2,4394)	1:71:A:ILE:HG23	1:80:A:PHE:HB3	13	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4351)	1:111:A:LEU:HD21	1:91:A:ILE:HD12	15	0.76
(2,4254)	1:45:A:LYS:HG3	1:47:A:ASP:HB3	19	0.76
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD12	5	0.76
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD13	16	0.76
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD13	3	0.76
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD13	3	0.76
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD11	3	0.76
(2,4131)	1:60:A:LEU:HA	1:24:A:ILE:HD12	11	0.76
(2,4105)	1:59:A:TYR:HE2	1:93:A:ILE:HD11	3	0.76
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD12	4	0.76
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD11	16	0.76
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD12	9	0.76
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG22	8	0.76
(2,3857)	1:66:A:ILE:HG21	1:49:A:VAL:HG21	9	0.76
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD22	5	0.76
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD23	19	0.76
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD23	18	0.76
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD23	11	0.76
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD23	15	0.76
(2,3689)	1:115:A:TYR:H	1:111:A:LEU:HD23	1	0.76
(2,3685)	1:27:A:ALA:H	1:49:A:VAL:HG23	5	0.76
(2,3247)	1:60:A:LEU:HD22	1:89:A:LYS:HB3	8	0.76
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	13	0.76
(2,2873)	1:91:A:ILE:HD12	1:87:A:ASN:HB2	13	0.76
(2,2496)	1:32:A:LEU:HB2	1:30:A:GLY:HA2	4	0.76
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	9	0.76
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	10	0.76
(2,2194)	1:28:A:LEU:HD12	1:54:A:SER:HA	1	0.76
(2,1666)	1:121:A:ILE:HD11	1:121:A:ILE:H	6	0.76
(2,1660)	1:130:A:THR:HG22	1:132:A:GLU:H	2	0.76
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	20	0.76
(2,1497)	1:81:A:VAL:HG11	1:83:A:GLY:H	12	0.76
(2,1497)	1:81:A:VAL:HG11	1:83:A:GLY:H	18	0.76
(2,1486)	1:69:A:ILE:HG13	1:83:A:GLY:H	18	0.76
(2,1402)	1:99:A:ILE:HG21	1:101:A:ASN:HD22	8	0.76
(2,1398)	1:111:A:LEU:HD23	1:114:A:GLU:H	1	0.76
(2,1389)	1:106:A:VAL:HG13	1:105:A:ASN:HD21	7	0.76
(2,1257)	1:108:A:VAL:HG13	1:113:A:ARG:H	4	0.76
(2,1051)	1:106:A:VAL:HG23	1:109:A:GLU:H	13	0.76
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	9	0.76
(2,596)	1:28:A:LEU:HD12	1:50:A:GLU:H	7	0.76
(2,596)	1:28:A:LEU:HD13	1:50:A:GLU:H	8	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4300)	1:65:A:LYS:HE3	1:63:A:LEU:HD21	16	0.75
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	4	0.75
(2,4254)	1:46:A:LYS:HG2	1:47:A:ASP:HB3	11	0.75
(2,4222)	1:75:A:GLU:HB3	1:73:A:SER:HB3	12	0.75
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD11	9	0.75
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD13	12	0.75
(2,4157)	1:88:A:LYS:HA	1:103:A:ILE:HD12	13	0.75
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD11	2	0.75
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD11	9	0.75
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD12	17	0.75
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD13	14	0.75
(2,4006)	1:80:A:PHE:HB3	1:99:A:ILE:HG21	10	0.75
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD22	4	0.75
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD22	12	0.75
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD22	14	0.75
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD21	4	0.75
(2,3685)	1:27:A:ALA:H	1:49:A:VAL:HG22	12	0.75
(2,3409)	1:79:A:TYR:HD2	1:123:A:LEU:HD21	7	0.75
(2,2873)	1:91:A:ILE:HD12	1:87:A:ASN:HB2	3	0.75
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	12	0.75
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	3	0.75
(2,1896)	1:60:A:LEU:HD13	1:93:A:ILE:HA	3	0.75
(2,1610)	1:95:A:LEU:HD21	1:110:A:LYS:H	8	0.75
(2,1610)	1:95:A:LEU:HD21	1:110:A:LYS:H	20	0.75
(2,1557)	1:24:A:ILE:HD12	1:61:A:TRP:HE1	4	0.75
(2,1398)	1:119:A:ILE:HD11	1:114:A:GLU:H	9	0.75
(2,1066)	1:99:A:ILE:HD12	1:97:A:ARG:H	8	0.75
(2,665)	1:115:A:TYR:HE1	1:112:A:LEU:H	12	0.75
(2,596)	1:28:A:LEU:HD12	1:50:A:GLU:H	14	0.75
(2,596)	1:28:A:LEU:HD12	1:50:A:GLU:H	20	0.75
(2,316)	1:26:A:ASP:HB3	1:32:A:LEU:H	13	0.75
(2,237)	1:90:A:ALA:HB3	1:93:A:ILE:H	3	0.75
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	14	0.75
(2,4689)	1:123:A:LEU:HD23	1:79:A:TYR:HD1	4	0.74
(2,4351)	1:111:A:LEU:HD21	1:91:A:ILE:HD11	19	0.74
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD12	7	0.74
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	6	0.74
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB2	7	0.74
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB2	9	0.74
(2,4222)	1:71:A:ILE:HB	1:73:A:SER:HB2	18	0.74
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD12	8	0.74
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD12	6	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD11	9	0.74
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD13	15	0.74
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD12	13	0.74
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG21	18	0.74
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD13	12	0.74
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD11	15	0.74
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD13	16	0.74
(2,4161)	1:89:A:LYS:HE2	1:93:A:ILE:HD13	15	0.74
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD11	18	0.74
(2,4107)	1:41:A:TYR:HD1	1:34:A:ILE:HD12	20	0.74
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD13	17	0.74
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD12	1	0.74
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD23	1	0.74
(2,3609)	1:13:A:ILE:HG13	1:125:A:PRO:HG2	15	0.74
(2,3409)	1:79:A:TYR:HD1	1:123:A:LEU:HD21	5	0.74
(2,3361)	1:87:A:ASN:HD22	1:64:A:VAL:HG22	10	0.74
(2,3333)	1:115:A:TYR:H	1:52:A:LEU:HD21	7	0.74
(2,2382)	1:103:A:ILE:HG21	1:107:A:ASP:HA	20	0.74
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	15	0.74
(2,1677)	1:65:A:LYS:HE2	1:23:A:THR:HB	3	0.74
(2,1666)	1:121:A:ILE:HD13	1:121:A:ILE:H	14	0.74
(2,1666)	1:121:A:ILE:HD11	1:121:A:ILE:H	19	0.74
(2,1660)	1:130:A:THR:HG23	1:132:A:GLU:H	4	0.74
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	5	0.74
(2,1497)	1:81:A:VAL:HG13	1:83:A:GLY:H	14	0.74
(2,1257)	1:108:A:VAL:HG12	1:113:A:ARG:H	10	0.74
(2,1257)	1:108:A:VAL:HG11	1:113:A:ARG:H	19	0.74
(2,1256)	1:24:A:ILE:HG21	1:54:A:SER:H	12	0.74
(2,1075)	1:52:A:LEU:HD21	1:115:A:TYR:H	7	0.74
(2,1066)	1:99:A:ILE:HD13	1:97:A:ARG:H	17	0.74
(2,1051)	1:106:A:VAL:HG22	1:109:A:GLU:H	4	0.74
(2,1051)	1:106:A:VAL:HG21	1:109:A:GLU:H	9	0.74
(2,600)	1:91:A:ILE:HD12	1:69:A:ILE:H	5	0.74
(2,596)	1:28:A:LEU:HD12	1:50:A:GLU:H	11	0.74
(2,596)	1:28:A:LEU:HD12	1:50:A:GLU:H	19	0.74
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	9	0.74
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE1	15	0.73
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE2	15	0.73
(2,4689)	1:123:A:LEU:HD23	1:79:A:TYR:HD1	8	0.73
(2,4551)	1:69:A:ILE:HD12	1:120:A:PHE:HE2	6	0.73
(2,4518)	1:76:A:ILE:HD11	1:80:A:PHE:HZ	19	0.73
(2,4474)	1:36:A:LEU:HD23	1:21:A:TYR:HD1	16	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD13	17	0.73
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD11	13	0.73
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD13	7	0.73
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD13	8	0.73
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG21	11	0.73
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG23	2	0.73
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG23	12	0.73
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD21	11	0.73
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD21	13	0.73
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD23	12	0.73
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG13	15	0.73
(2,3501)	1:112:A:LEU:HA	1:121:A:ILE:HG13	1	0.73
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	2	0.73
(2,3409)	1:79:A:TYR:HD2	1:123:A:LEU:HD21	17	0.73
(2,3361)	1:87:A:ASN:HD22	1:64:A:VAL:HG23	12	0.73
(2,3333)	1:94:A:LEU:H	1:52:A:LEU:HD11	2	0.73
(2,3280)	1:79:A:TYR:H	1:104:A:LEU:HG	12	0.73
(2,2865)	1:76:A:ILE:HG23	1:105:A:ASN:HB2	12	0.73
(2,2560)	1:120:A:PHE:HE1	1:34:A:ILE:HB	16	0.73
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	19	0.73
(2,2174)	1:99:A:ILE:HD11	1:89:A:LYS:HA	5	0.73
(2,1885)	1:123:A:LEU:HD21	1:125:A:PRO:HA	15	0.73
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	1	0.73
(2,1666)	1:121:A:ILE:HD13	1:121:A:ILE:H	9	0.73
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	16	0.73
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	7	0.73
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	17	0.73
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	18	0.73
(2,1501)	1:95:A:LEU:HD11	1:96:A:GLY:H	14	0.73
(2,1497)	1:81:A:VAL:HG12	1:83:A:GLY:H	13	0.73
(2,1486)	1:69:A:ILE:HG13	1:83:A:GLY:H	4	0.73
(2,1398)	1:119:A:ILE:HD13	1:114:A:GLU:H	4	0.73
(2,1398)	1:119:A:ILE:HD11	1:114:A:GLU:H	10	0.73
(2,1051)	1:106:A:VAL:HG21	1:109:A:GLU:H	11	0.73
(2,665)	1:115:A:TYR:HE2	1:112:A:LEU:H	2	0.73
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	18	0.73
(2,596)	1:28:A:LEU:HD12	1:50:A:GLU:H	1	0.73
(2,510)	1:59:A:TYR:HB2	1:64:A:VAL:H	4	0.73
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	4	0.73
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	8	0.73
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	18	0.73
(2,168)	1:119:A:ILE:HG23	1:122:A:ILE:H	9	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE1	19	0.72
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE2	19	0.72
(2,4518)	1:76:A:ILE:HD13	1:80:A:PHE:HZ	9	0.72
(2,4458)	1:20:A:GLU:HB2	1:21:A:TYR:HD1	9	0.72
(2,4373)	1:130:A:THR:HG22	1:134:A:GLU:HB3	8	0.72
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG23	4	0.72
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD13	12	0.72
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD12	13	0.72
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG22	19	0.72
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD12	9	0.72
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD13	10	0.72
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD11	15	0.72
(2,4107)	1:41:A:TYR:HD1	1:34:A:ILE:HD13	10	0.72
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD12	17	0.72
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG21	5	0.72
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG21	12	0.72
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD23	6	0.72
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD21	17	0.72
(2,2874)	1:118:A:LEU:HD21	1:48:A:GLU:HG3	8	0.72
(2,1899)	1:76:A:ILE:HD11	1:73:A:SER:HB2	1	0.72
(2,1896)	1:60:A:LEU:HD11	1:93:A:ILE:HA	5	0.72
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	10	0.72
(2,1497)	1:81:A:VAL:HG12	1:83:A:GLY:H	5	0.72
(2,1497)	1:81:A:VAL:HG12	1:83:A:GLY:H	8	0.72
(2,1497)	1:81:A:VAL:HG11	1:83:A:GLY:H	15	0.72
(2,1497)	1:81:A:VAL:HG13	1:83:A:GLY:H	17	0.72
(2,1404)	1:122:A:ILE:HD12	1:37:A:ASN:HD22	13	0.72
(2,1389)	1:106:A:VAL:HG12	1:105:A:ASN:HD21	15	0.72
(2,1228)	1:123:A:LEU:HD22	1:124:A:SER:H	20	0.72
(2,1066)	1:99:A:ILE:HD12	1:97:A:ARG:H	5	0.72
(2,596)	1:28:A:LEU:HD13	1:50:A:GLU:H	9	0.72
(2,596)	1:28:A:LEU:HD13	1:50:A:GLU:H	10	0.72
(2,596)	1:28:A:LEU:HD12	1:50:A:GLU:H	13	0.72
(2,510)	1:65:A:LYS:HE2	1:64:A:VAL:H	10	0.72
(2,248)	1:36:A:LEU:HD11	1:36:A:LEU:H	7	0.72
(2,4689)	1:123:A:LEU:HD21	1:79:A:TYR:HD1	18	0.71
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD2	20	0.71
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD2	12	0.71
(2,4394)	1:71:A:ILE:HG22	1:80:A:PHE:HB3	14	0.71
(2,4381)	1:133:A:THR:HG21	1:137:A:GLU:HG2	17	0.71
(2,4373)	1:130:A:THR:HG21	1:134:A:GLU:HB3	5	0.71
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB2	5	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4243)	1:102:A:VAL:HG22	1:104:A:LEU:HA	16	0.71
(2,4190)	1:64:A:VAL:HG23	1:24:A:ILE:HG23	17	0.71
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG21	14	0.71
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD12	18	0.71
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD12	7	0.71
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG21	14	0.71
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG22	14	0.71
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	20	0.71
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB2	18	0.71
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG21	14	0.71
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG11	2	0.71
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD23	18	0.71
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD23	3	0.71
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG12	6	0.71
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD22	3	0.71
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD23	5	0.71
(2,3463)	1:87:A:ASN:HA	1:88:A:LYS:HG3	12	0.71
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	1	0.71
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	1	0.71
(2,3072)	1:88:A:LYS:H	1:85:A:GLN:HG2	15	0.71
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	6	0.71
(2,2651)	1:95:A:LEU:HD23	1:110:A:LYS:HE3	11	0.71
(2,2382)	1:28:A:LEU:HD21	1:47:A:ASP:HA	12	0.71
(2,2194)	1:58:A:LEU:HD22	1:54:A:SER:HA	8	0.71
(2,2174)	1:60:A:LEU:HG	1:59:A:TYR:HA	4	0.71
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	6	0.71
(2,1896)	1:60:A:LEU:HD11	1:93:A:ILE:HA	10	0.71
(2,1896)	1:60:A:LEU:HD11	1:93:A:ILE:HA	13	0.71
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	11	0.71
(2,1626)	1:135:A:LEU:HD22	1:136:A:SER:H	6	0.71
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	10	0.71
(2,1486)	1:69:A:ILE:HG13	1:83:A:GLY:H	17	0.71
(2,1066)	1:99:A:ILE:HD11	1:97:A:ARG:H	11	0.71
(2,1051)	1:106:A:VAL:HG22	1:109:A:GLU:H	12	0.71
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	11	0.71
(2,600)	1:91:A:ILE:HD12	1:69:A:ILE:H	2	0.71
(2,245)	1:44:A:ILE:HD12	1:44:A:ILE:H	6	0.71
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	20	0.71
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE1	13	0.7
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	15	0.7
(2,4457)	1:20:A:GLU:HG3	1:21:A:TYR:HD1	8	0.7
(2,4457)	1:43:A:GLU:HG3	1:41:A:TYR:HD1	20	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4394)	1:71:A:ILE:HG21	1:80:A:PHE:HB3	7	0.7
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB2	7	0.7
(2,4300)	1:65:A:LYS:HE3	1:63:A:LEU:HD22	14	0.7
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD23	2	0.7
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	20	0.7
(2,4190)	1:64:A:VAL:HG21	1:24:A:ILE:HG21	14	0.7
(2,4107)	1:21:A:TYR:HD1	1:34:A:ILE:HD11	16	0.7
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD13	1	0.7
(2,4093)	1:120:A:PHE:HD1	1:69:A:ILE:HD12	20	0.7
(2,4092)	1:14:A:PHE:HD1	1:122:A:ILE:HD11	14	0.7
(2,4072)	1:94:A:LEU:H	1:93:A:ILE:HD13	7	0.7
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD12	18	0.7
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG21	17	0.7
(2,3966)	1:98:A:GLU:HA	1:99:A:ILE:HG21	16	0.7
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG12	14	0.7
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD21	16	0.7
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD21	17	0.7
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD21	13	0.7
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG21	4	0.7
(2,3280)	1:79:A:TYR:H	1:104:A:LEU:HG	6	0.7
(2,2873)	1:91:A:ILE:HD12	1:87:A:ASN:HB2	2	0.7
(2,2382)	1:103:A:ILE:HG13	1:107:A:ASP:HA	1	0.7
(2,2382)	1:103:A:ILE:HG22	1:107:A:ASP:HA	17	0.7
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	1	0.7
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	19	0.7
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	7	0.7
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	8	0.7
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	9	0.7
(2,1666)	1:121:A:ILE:HD13	1:121:A:ILE:H	8	0.7
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	9	0.7
(2,1557)	1:24:A:ILE:HD11	1:61:A:TRP:HE1	14	0.7
(2,1557)	1:24:A:ILE:HD13	1:61:A:TRP:HE1	17	0.7
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	4	0.7
(2,1501)	1:95:A:LEU:HD13	1:96:A:GLY:H	3	0.7
(2,1501)	1:95:A:LEU:HD13	1:96:A:GLY:H	17	0.7
(2,1240)	1:112:A:LEU:HD12	1:113:A:ARG:H	17	0.7
(2,1228)	1:122:A:ILE:HG21	1:124:A:SER:H	14	0.7
(2,1219)	1:45:A:LYS:HG3	1:47:A:ASP:H	2	0.7
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	16	0.7
(2,596)	1:28:A:LEU:HD12	1:50:A:GLU:H	3	0.7
(2,596)	1:28:A:LEU:HD13	1:50:A:GLU:H	16	0.7
(2,344)	1:108:A:VAL:HG11	1:71:A:ILE:H	4	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,245)	1:44:A:ILE:HG23	1:44:A:ILE:H	5	0.7
(2,245)	1:32:A:LEU:HD21	1:44:A:ILE:H	9	0.7
(2,4474)	1:36:A:LEU:HD23	1:41:A:TYR:HD1	14	0.69
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD2	14	0.69
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB1	2	0.69
(2,4300)	1:65:A:LYS:HE2	1:63:A:LEU:HD22	2	0.69
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD22	8	0.69
(2,4243)	1:102:A:VAL:HG23	1:104:A:LEU:HA	2	0.69
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD12	2	0.69
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD12	8	0.69
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD12	11	0.69
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD12	7	0.69
(2,4093)	1:120:A:PHE:HD1	1:122:A:ILE:HD13	1	0.69
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD12	14	0.69
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD22	10	0.69
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD21	17	0.69
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG21	8	0.69
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD11	19	0.69
(2,2652)	1:95:A:LEU:HD22	1:107:A:ASP:HB2	17	0.69
(2,2469)	1:60:A:LEU:HG	1:57:A:PRO:HD3	20	0.69
(2,2382)	1:103:A:ILE:HG22	1:107:A:ASP:HA	6	0.69
(2,2163)	1:102:A:VAL:HG23	1:103:A:ILE:HA	13	0.69
(2,1896)	1:60:A:LEU:HD12	1:93:A:ILE:HA	4	0.69
(2,1896)	1:60:A:LEU:HD13	1:93:A:ILE:HA	11	0.69
(2,1666)	1:122:A:ILE:HD13	1:121:A:ILE:H	15	0.69
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	11	0.69
(2,1550)	1:50:A:GLU:HG2	1:46:A:LYS:H	16	0.69
(2,1501)	1:95:A:LEU:HD11	1:96:A:GLY:H	12	0.69
(2,1256)	1:24:A:ILE:HG23	1:54:A:SER:H	8	0.69
(2,1051)	1:106:A:VAL:HG23	1:109:A:GLU:H	7	0.69
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	1	0.69
(2,610)	1:24:A:ILE:HG23	1:63:A:LEU:H	7	0.69
(2,596)	1:28:A:LEU:HD11	1:50:A:GLU:H	2	0.69
(2,596)	1:28:A:LEU:HD11	1:50:A:GLU:H	12	0.69
(2,596)	1:28:A:LEU:HD12	1:50:A:GLU:H	18	0.69
(2,331)	1:31:A:LYS:HD3	1:32:A:LEU:H	11	0.69
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	12	0.69
(2,248)	1:36:A:LEU:HD11	1:36:A:LEU:H	10	0.69
(2,248)	1:36:A:LEU:HD12	1:36:A:LEU:H	12	0.69
(2,248)	1:36:A:LEU:HD13	1:36:A:LEU:H	18	0.69
(2,248)	1:36:A:LEU:HD11	1:36:A:LEU:H	19	0.69
(2,245)	1:44:A:ILE:HD13	1:44:A:ILE:H	19	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	13	0.69
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE1	10	0.68
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE2	10	0.68
(2,4689)	1:123:A:LEU:HD23	1:79:A:TYR:HD2	17	0.68
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	16	0.68
(2,4254)	1:46:A:LYS:HG2	1:47:A:ASP:HB3	8	0.68
(2,4178)	1:64:A:VAL:HB	1:24:A:ILE:HG22	6	0.68
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD11	13	0.68
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD11	3	0.68
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG22	17	0.68
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG21	11	0.68
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	18	0.68
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	19	0.68
(2,3838)	1:31:A:LYS:HG2	1:22:A:VAL:HG12	13	0.68
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD21	6	0.68
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD21	1	0.68
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD22	13	0.68
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD21	4	0.68
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD22	16	0.68
(2,3609)	1:13:A:ILE:HG13	1:125:A:PRO:HG2	11	0.68
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD21	17	0.68
(2,3501)	1:112:A:LEU:HA	1:121:A:ILE:HG13	11	0.68
(2,3409)	1:79:A:TYR:HD1	1:123:A:LEU:HD21	15	0.68
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	4	0.68
(2,3280)	1:79:A:TYR:H	1:104:A:LEU:HG	4	0.68
(2,3072)	1:88:A:LYS:H	1:85:A:GLN:HG2	3	0.68
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	17	0.68
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	2	0.68
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	13	0.68
(2,2863)	1:22:A:VAL:HG13	1:26:A:ASP:HB3	19	0.68
(2,2560)	1:21:A:TYR:HE2	1:34:A:ILE:HB	17	0.68
(2,2382)	1:103:A:ILE:HG23	1:107:A:ASP:HA	19	0.68
(2,2194)	1:28:A:LEU:HD13	1:54:A:SER:HA	6	0.68
(2,2175)	1:94:A:LEU:HD22	1:52:A:LEU:HA	14	0.68
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	9	0.68
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	14	0.68
(2,1899)	1:76:A:ILE:HG23	1:73:A:SER:HB3	5	0.68
(2,1896)	1:60:A:LEU:HD12	1:93:A:ILE:HA	17	0.68
(2,1885)	1:123:A:LEU:HD22	1:125:A:PRO:HA	3	0.68
(2,1885)	1:123:A:LEU:HD23	1:125:A:PRO:HA	11	0.68
(2,1885)	1:123:A:LEU:HD22	1:125:A:PRO:HA	16	0.68
(2,1610)	1:95:A:LEU:HD23	1:110:A:LYS:H	9	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1610)	1:95:A:LEU:HD22	1:110:A:LYS:H	15	0.68
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	19	0.68
(2,1557)	1:24:A:ILE:HD12	1:61:A:TRP:HE1	18	0.68
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	19	0.68
(2,1501)	1:95:A:LEU:HD12	1:96:A:GLY:H	4	0.68
(2,1404)	1:69:A:ILE:HD13	1:37:A:ASN:HD22	16	0.68
(2,1226)	1:91:A:ILE:HG23	1:95:A:LEU:H	4	0.68
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	20	0.68
(2,600)	1:91:A:ILE:HD12	1:69:A:ILE:H	6	0.68
(2,550)	1:60:A:LEU:HB2	1:63:A:LEU:H	5	0.68
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	5	0.68
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	19	0.68
(2,4518)	1:76:A:ILE:HD13	1:80:A:PHE:HZ	11	0.67
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD1	16	0.67
(2,4331)	1:61:A:TRP:HB2	1:24:A:ILE:HD11	12	0.67
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB2	10	0.67
(2,4254)	1:45:A:LYS:HG3	1:47:A:ASP:HB3	17	0.67
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD13	16	0.67
(2,4120)	1:21:A:TYR:HA	1:34:A:ILE:HD11	20	0.67
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD13	1	0.67
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD13	3	0.67
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD13	20	0.67
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG21	4	0.67
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG22	3	0.67
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	10	0.67
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG21	12	0.67
(2,3857)	1:66:A:ILE:HG21	1:49:A:VAL:HG21	15	0.67
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD23	17	0.67
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD22	13	0.67
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD22	15	0.67
(2,3299)	1:44:A:ILE:H	1:33:A:LYS:HG2	4	0.67
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	11	0.67
(2,2174)	1:99:A:ILE:HD11	1:89:A:LYS:HA	3	0.67
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	13	0.67
(2,1677)	1:65:A:LYS:HE2	1:23:A:THR:HB	10	0.67
(2,1666)	1:121:A:ILE:HD13	1:121:A:ILE:H	4	0.67
(2,1610)	1:95:A:LEU:HD21	1:110:A:LYS:H	4	0.67
(2,1610)	1:95:A:LEU:HD21	1:110:A:LYS:H	7	0.67
(2,1610)	1:95:A:LEU:HD21	1:110:A:LYS:H	11	0.67
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	18	0.67
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	19	0.67
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	6	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	8	0.67
(2,1497)	1:81:A:VAL:HG12	1:83:A:GLY:H	2	0.67
(2,1486)	1:69:A:ILE:HG13	1:83:A:GLY:H	14	0.67
(2,1401)	1:106:A:VAL:HG23	1:105:A:ASN:HD22	10	0.67
(2,1314)	1:100:A:SER:HB2	1:101:A:ASN:HD21	20	0.67
(2,1257)	1:108:A:VAL:HG12	1:113:A:ARG:H	9	0.67
(2,1228)	1:122:A:ILE:HG22	1:124:A:SER:H	15	0.67
(2,1222)	1:33:A:LYS:HD2	1:41:A:TYR:H	16	0.67
(2,1036)	1:34:A:ILE:HB	1:33:A:LYS:H	6	0.67
(2,1036)	1:43:A:GLU:HG2	1:33:A:LYS:H	18	0.67
(2,607)	1:66:A:ILE:HG23	1:64:A:VAL:H	8	0.67
(2,598)	1:24:A:ILE:HG22	1:52:A:LEU:H	9	0.67
(2,331)	1:33:A:LYS:HB3	1:32:A:LEU:H	5	0.67
(2,248)	1:36:A:LEU:HD11	1:36:A:LEU:H	5	0.67
(2,237)	1:90:A:ALA:HB1	1:93:A:ILE:H	2	0.67
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	10	0.67
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	11	0.67
(2,235)	1:31:A:LYS:HB3	1:27:A:ALA:H	5	0.67
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	16	0.67
(2,4551)	1:69:A:ILE:HD13	1:120:A:PHE:HE2	19	0.66
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD1	5	0.66
(2,4457)	1:20:A:GLU:HG3	1:21:A:TYR:HD2	4	0.66
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB3	8	0.66
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB3	14	0.66
(2,4289)	1:53:A:SER:HB2	1:52:A:LEU:HD21	19	0.66
(2,4209)	1:87:A:ASN:HA	1:91:A:ILE:HD12	3	0.66
(2,4131)	1:64:A:VAL:HA	1:24:A:ILE:HD12	6	0.66
(2,4120)	1:21:A:TYR:HA	1:34:A:ILE:HD13	4	0.66
(2,4107)	1:21:A:TYR:HD1	1:34:A:ILE:HD11	1	0.66
(2,4107)	1:41:A:TYR:HD2	1:34:A:ILE:HD11	7	0.66
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD13	8	0.66
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD12	13	0.66
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD11	11	0.66
(2,4064)	1:70:A:PHE:H	1:69:A:ILE:HD12	16	0.66
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG22	19	0.66
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG22	20	0.66
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG23	1	0.66
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG22	8	0.66
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG22	7	0.66
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG11	19	0.66
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG12	10	0.66
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD21	3	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD21	7	0.66
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD23	19	0.66
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD21	20	0.66
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD22	10	0.66
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD22	14	0.66
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	18	0.66
(2,3501)	1:112:A:LEU:HA	1:121:A:ILE:HG13	19	0.66
(2,3361)	1:87:A:ASN:HD22	1:64:A:VAL:HG21	16	0.66
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG21	18	0.66
(2,2842)	1:25:A:LYS:HB2	1:26:A:ASP:HB2	17	0.66
(2,2382)	1:103:A:ILE:HG23	1:107:A:ASP:HA	15	0.66
(2,2163)	1:102:A:VAL:HG22	1:103:A:ILE:HA	4	0.66
(2,2143)	1:133:A:THR:HG22	1:134:A:GLU:HA	8	0.66
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	3	0.66
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	16	0.66
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	16	0.66
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	6	0.66
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	11	0.66
(2,1401)	1:106:A:VAL:HG21	1:105:A:ASN:HD22	12	0.66
(2,1256)	1:24:A:ILE:HG21	1:54:A:SER:H	1	0.66
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	1	0.66
(2,607)	1:66:A:ILE:HG22	1:64:A:VAL:H	9	0.66
(2,596)	1:28:A:LEU:HD11	1:50:A:GLU:H	17	0.66
(2,550)	1:60:A:LEU:HB2	1:63:A:LEU:H	8	0.66
(2,168)	1:119:A:ILE:HG22	1:122:A:ILE:H	2	0.66
(2,77)	1:56:A:ILE:HD13	1:61:A:TRP:HE1	8	0.66
(2,33)	1:46:A:LYS:HD2	1:46:A:LYS:H	16	0.66
(2,4551)	1:34:A:ILE:HG23	1:120:A:PHE:HE2	1	0.65
(2,4518)	1:102:A:VAL:HG21	1:80:A:PHE:HZ	10	0.65
(2,4518)	1:102:A:VAL:HG21	1:80:A:PHE:HZ	16	0.65
(2,4501)	1:10:A:LEU:HB3	1:14:A:PHE:HE1	7	0.65
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD1	5	0.65
(2,4458)	1:20:A:GLU:HB2	1:21:A:TYR:HD2	20	0.65
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB1	12	0.65
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB1	15	0.65
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB1	19	0.65
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD12	3	0.65
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD11	8	0.65
(2,4107)	1:21:A:TYR:HD2	1:34:A:ILE:HD13	4	0.65
(2,4107)	1:21:A:TYR:HD1	1:34:A:ILE:HD12	18	0.65
(2,4093)	1:120:A:PHE:HD2	1:122:A:ILE:HD12	9	0.65
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD13	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD12	16	0.65
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD11	17	0.65
(2,3905)	1:80:A:PHE:HE1	1:102:A:VAL:HG21	14	0.65
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG21	8	0.65
(2,3685)	1:27:A:ALA:H	1:49:A:VAL:HG21	7	0.65
(2,3635)	1:52:A:LEU:HD12	1:56:A:ILE:HG12	10	0.65
(2,3501)	1:112:A:LEU:HA	1:121:A:ILE:HG13	9	0.65
(2,3501)	1:112:A:LEU:HA	1:121:A:ILE:HG13	14	0.65
(2,3409)	1:59:A:TYR:HE1	1:60:A:LEU:HD21	6	0.65
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG22	1	0.65
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD11	9	0.65
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	19	0.65
(2,2863)	1:22:A:VAL:HG12	1:26:A:ASP:HB3	11	0.65
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	16	0.65
(2,2863)	1:22:A:VAL:HG12	1:26:A:ASP:HB3	17	0.65
(2,2842)	1:25:A:LYS:HB2	1:26:A:ASP:HB2	12	0.65
(2,2194)	1:58:A:LEU:HD22	1:54:A:SER:HA	12	0.65
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	7	0.65
(2,1877)	1:137:A:GLU:HB2	1:136:A:SER:HB2	20	0.65
(2,1677)	1:65:A:LYS:HE2	1:23:A:THR:HB	2	0.65
(2,1666)	1:122:A:ILE:HD13	1:121:A:ILE:H	17	0.65
(2,1660)	1:130:A:THR:HG23	1:132:A:GLU:H	17	0.65
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	2	0.65
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	2	0.65
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	3	0.65
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	12	0.65
(2,1501)	1:95:A:LEU:HD11	1:96:A:GLY:H	10	0.65
(2,1501)	1:95:A:LEU:HD13	1:96:A:GLY:H	19	0.65
(2,1398)	1:119:A:ILE:HD12	1:114:A:GLU:H	8	0.65
(2,1226)	1:95:A:LEU:HD11	1:95:A:LEU:H	13	0.65
(2,1226)	1:95:A:LEU:HD12	1:95:A:LEU:H	15	0.65
(2,852)	1:88:A:LYS:HG3	1:87:A:ASN:H	13	0.65
(2,761)	1:101:A:ASN:HB3	1:103:A:ILE:H	12	0.65
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	20	0.65
(2,607)	1:66:A:ILE:HG21	1:64:A:VAL:H	1	0.65
(2,596)	1:28:A:LEU:HD13	1:50:A:GLU:H	6	0.65
(2,560)	1:95:A:LEU:HD12	1:104:A:LEU:H	19	0.65
(2,510)	1:59:A:TYR:HB2	1:64:A:VAL:H	8	0.65
(2,331)	1:33:A:LYS:HB3	1:32:A:LEU:H	8	0.65
(2,331)	1:33:A:LYS:HB3	1:32:A:LEU:H	9	0.65
(2,248)	1:36:A:LEU:HD12	1:36:A:LEU:H	9	0.65
(2,248)	1:36:A:LEU:HD11	1:36:A:LEU:H	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,245)	1:32:A:LEU:HD22	1:44:A:ILE:H	13	0.65
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	5	0.65
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	15	0.65
(2,235)	1:25:A:LYS:HB3	1:27:A:ALA:H	6	0.65
(2,235)	1:25:A:LYS:HB3	1:27:A:ALA:H	14	0.65
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	15	0.65
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE1	1	0.64
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE2	1	0.64
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE1	3	0.64
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE2	3	0.64
(2,4689)	1:123:A:LEU:HD21	1:79:A:TYR:HD2	10	0.64
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE1	5	0.64
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	2	0.64
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	20	0.64
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD12	4	0.64
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD13	9	0.64
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD11	13	0.64
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD12	11	0.64
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD11	12	0.64
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB2	5	0.64
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	13	0.64
(2,4249)	1:94:A:LEU:HD11	1:55:A:ARG:HD3	7	0.64
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD11	10	0.64
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD12	19	0.64
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD13	12	0.64
(2,4107)	1:41:A:TYR:HD2	1:34:A:ILE:HD13	9	0.64
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD11	17	0.64
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD13	1	0.64
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG22	3	0.64
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG23	19	0.64
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG23	17	0.64
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG21	13	0.64
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG21	13	0.64
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG13	11	0.64
(2,3788)	1:57:A:PRO:HD2	1:94:A:LEU:HD21	13	0.64
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD21	7	0.64
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD23	5	0.64
(2,3685)	1:27:A:ALA:H	1:49:A:VAL:HG23	3	0.64
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD22	11	0.64
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD21	20	0.64
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	14	0.64
(2,2560)	1:21:A:TYR:HE1	1:34:A:ILE:HB	19	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2382)	1:103:A:ILE:HG23	1:107:A:ASP:HA	9	0.64
(2,2382)	1:103:A:ILE:HG13	1:107:A:ASP:HA	11	0.64
(2,2364)	1:93:A:ILE:HG22	1:90:A:ALA:HA	7	0.64
(2,2174)	1:99:A:ILE:HD13	1:89:A:LYS:HA	10	0.64
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	5	0.64
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	9	0.64
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	10	0.64
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	14	0.64
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	5	0.64
(2,1501)	1:95:A:LEU:HD12	1:96:A:GLY:H	1	0.64
(2,1501)	1:95:A:LEU:HD12	1:96:A:GLY:H	5	0.64
(2,1501)	1:95:A:LEU:HD12	1:96:A:GLY:H	11	0.64
(2,1257)	1:108:A:VAL:HG11	1:113:A:ARG:H	8	0.64
(2,1225)	1:95:A:LEU:HD21	1:95:A:LEU:H	1	0.64
(2,1051)	1:106:A:VAL:HG21	1:109:A:GLU:H	8	0.64
(2,863)	1:122:A:ILE:HG22	1:13:A:ILE:H	11	0.64
(2,550)	1:24:A:ILE:HG13	1:63:A:LEU:H	1	0.64
(2,348)	1:58:A:LEU:HD23	1:61:A:TRP:H	12	0.64
(2,344)	1:108:A:VAL:HG12	1:71:A:ILE:H	15	0.64
(2,248)	1:36:A:LEU:HD11	1:36:A:LEU:H	2	0.64
(2,245)	1:44:A:ILE:HD11	1:44:A:ILE:H	12	0.64
(2,77)	1:56:A:ILE:HD12	1:61:A:TRP:HE1	13	0.64
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE1	20	0.63
(2,4518)	1:102:A:VAL:HG22	1:80:A:PHE:HZ	5	0.63
(2,4518)	1:76:A:ILE:HD12	1:80:A:PHE:HZ	8	0.63
(2,4465)	1:118:A:LEU:HD11	1:115:A:TYR:HD2	12	0.63
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	3	0.63
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	6	0.63
(2,4377)	1:112:A:LEU:HD12	1:109:A:GLU:HG3	6	0.63
(2,4373)	1:130:A:THR:HG21	1:131:A:GLU:HB3	12	0.63
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD11	5	0.63
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD13	8	0.63
(2,4300)	1:65:A:LYS:HE2	1:63:A:LEU:HD22	9	0.63
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD13	4	0.63
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD13	7	0.63
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD13	5	0.63
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD12	15	0.63
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD11	19	0.63
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG21	8	0.63
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG22	3	0.63
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	7	0.63
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG21	16	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD21	10	0.63
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD22	11	0.63
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD23	1	0.63
(2,3681)	1:74:A:SER:H	1:126:A:THR:HG23	15	0.63
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD23	1	0.63
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD22	14	0.63
(2,3409)	1:59:A:TYR:HE2	1:60:A:LEU:HD21	4	0.63
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	1	0.63
(2,2863)	1:22:A:VAL:HG12	1:26:A:ASP:HB3	14	0.63
(2,2651)	1:22:A:VAL:HG11	1:31:A:LYS:HE3	13	0.63
(2,2542)	1:115:A:TYR:HD1	1:111:A:LEU:HB2	5	0.63
(2,2174)	1:99:A:ILE:HD11	1:89:A:LYS:HA	15	0.63
(2,2163)	1:102:A:VAL:HG21	1:103:A:ILE:HA	6	0.63
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	17	0.63
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	19	0.63
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	20	0.63
(2,1818)	1:80:A:PHE:HB2	1:81:A:VAL:HA	15	0.63
(2,1714)	1:131:A:GLU:HB2	1:130:A:THR:HB	6	0.63
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	8	0.63
(2,1557)	1:24:A:ILE:HD12	1:61:A:TRP:HE1	15	0.63
(2,1401)	1:106:A:VAL:HG21	1:105:A:ASN:HD22	14	0.63
(2,1226)	1:95:A:LEU:HD11	1:95:A:LEU:H	20	0.63
(2,1066)	1:99:A:ILE:HD11	1:97:A:ARG:H	14	0.63
(2,1051)	1:106:A:VAL:HG21	1:109:A:GLU:H	15	0.63
(2,607)	1:66:A:ILE:HG22	1:64:A:VAL:H	5	0.63
(2,600)	1:91:A:ILE:HD11	1:69:A:ILE:H	10	0.63
(2,600)	1:91:A:ILE:HD13	1:69:A:ILE:H	15	0.63
(2,248)	1:36:A:LEU:HD11	1:36:A:LEU:H	15	0.63
(2,245)	1:44:A:ILE:HD11	1:44:A:ILE:H	10	0.63
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	6	0.63
(2,77)	1:56:A:ILE:HD11	1:61:A:TRP:HE1	6	0.63
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE1	2	0.62
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE2	2	0.62
(2,4551)	1:122:A:ILE:HD12	1:120:A:PHE:HE2	16	0.62
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE2	4	0.62
(2,4469)	1:69:A:ILE:HD13	1:21:A:TYR:HD1	10	0.62
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD2	2	0.62
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD1	18	0.62
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	10	0.62
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD13	1	0.62
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD12	19	0.62
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB2	4	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB1	6	0.62
(2,4254)	1:46:A:LYS:HG2	1:47:A:ASP:HB3	15	0.62
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD12	10	0.62
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD13	12	0.62
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG21	16	0.62
(2,4000)	1:72:A:LYS:HE2	1:121:A:ILE:HG22	6	0.62
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG22	11	0.62
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG22	12	0.62
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG21	1	0.62
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG22	17	0.62
(2,3905)	1:80:A:PHE:HE1	1:102:A:VAL:HG22	6	0.62
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG22	5	0.62
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG22	10	0.62
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD22	1	0.62
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD22	13	0.62
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD23	1	0.62
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD23	12	0.62
(2,3685)	1:27:A:ALA:H	1:49:A:VAL:HG23	10	0.62
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD22	18	0.62
(2,3635)	1:52:A:LEU:HD12	1:56:A:ILE:HG12	2	0.62
(2,3409)	1:59:A:TYR:HE1	1:60:A:LEU:HD21	20	0.62
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	3	0.62
(2,2863)	1:22:A:VAL:HG12	1:26:A:ASP:HB3	15	0.62
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	20	0.62
(2,2382)	1:103:A:ILE:HG22	1:107:A:ASP:HA	7	0.62
(2,2364)	1:93:A:ILE:HG23	1:90:A:ALA:HA	19	0.62
(2,1899)	1:76:A:ILE:HG22	1:73:A:SER:HB2	16	0.62
(2,1896)	1:60:A:LEU:HD12	1:93:A:ILE:HA	19	0.62
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	5	0.62
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	18	0.62
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	8	0.62
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	20	0.62
(2,1557)	1:24:A:ILE:HD11	1:61:A:TRP:HE1	7	0.62
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	1	0.62
(2,1501)	1:95:A:LEU:HD11	1:96:A:GLY:H	13	0.62
(2,1501)	1:95:A:LEU:HD12	1:96:A:GLY:H	15	0.62
(2,1497)	1:81:A:VAL:HG13	1:83:A:GLY:H	6	0.62
(2,1256)	1:28:A:LEU:HD13	1:54:A:SER:H	5	0.62
(2,1240)	1:112:A:LEU:HD13	1:113:A:ARG:H	20	0.62
(2,1234)	1:94:A:LEU:HD23	1:56:A:ILE:H	2	0.62
(2,1226)	1:95:A:LEU:HD13	1:95:A:LEU:H	17	0.62
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,663)	1:115:A:TYR:HD1	1:112:A:LEU:H	13	0.62
(2,610)	1:24:A:ILE:HG23	1:63:A:LEU:H	5	0.62
(2,550)	1:60:A:LEU:HB2	1:63:A:LEU:H	14	0.62
(2,333)	1:56:A:ILE:HG21	1:61:A:TRP:H	1	0.62
(2,248)	1:36:A:LEU:HD11	1:36:A:LEU:H	17	0.62
(2,245)	1:44:A:ILE:HD13	1:44:A:ILE:H	17	0.62
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	20	0.62
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	18	0.62
(2,77)	1:56:A:ILE:HD13	1:61:A:TRP:HE1	4	0.62
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	6	0.62
(2,4551)	1:122:A:ILE:HD11	1:120:A:PHE:HE1	3	0.61
(2,4551)	1:69:A:ILE:HD13	1:120:A:PHE:HE1	10	0.61
(2,4518)	1:76:A:ILE:HD13	1:80:A:PHE:HZ	4	0.61
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD12	3	0.61
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD13	5	0.61
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD12	13	0.61
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD12	16	0.61
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD11	17	0.61
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG21	20	0.61
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD12	9	0.61
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD12	19	0.61
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD12	20	0.61
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD13	2	0.61
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD11	5	0.61
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD12	10	0.61
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG21	5	0.61
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG22	19	0.61
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG22	2	0.61
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG22	16	0.61
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD21	16	0.61
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD21	5	0.61
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD22	9	0.61
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG12	17	0.61
(2,3705)	1:14:A:PHE:HD2	1:10:A:LEU:HD22	15	0.61
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD21	18	0.61
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD22	9	0.61
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	4	0.61
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	5	0.61
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	11	0.61
(2,3361)	1:87:A:ASN:HD22	1:64:A:VAL:HG23	7	0.61
(2,3247)	1:60:A:LEU:HD23	1:89:A:LYS:HB3	6	0.61
(2,3009)	1:34:A:ILE:HG22	1:20:A:GLU:HG2	2	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	7	0.61
(2,2865)	1:76:A:ILE:HG21	1:105:A:ASN:HB2	7	0.61
(2,2473)	1:69:A:ILE:HD12	1:18:A:PRO:HD3	3	0.61
(2,2375)	1:104:A:LEU:HD22	1:78:A:GLU:HA	6	0.61
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	16	0.61
(2,1818)	1:80:A:PHE:HB2	1:81:A:VAL:HA	6	0.61
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	2	0.61
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	13	0.61
(2,1557)	1:24:A:ILE:HD12	1:61:A:TRP:HE1	2	0.61
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	5	0.61
(2,1398)	1:119:A:ILE:HD12	1:114:A:GLU:H	6	0.61
(2,1398)	1:119:A:ILE:HD12	1:114:A:GLU:H	15	0.61
(2,1256)	1:24:A:ILE:HG21	1:54:A:SER:H	11	0.61
(2,1234)	1:94:A:LEU:HD22	1:56:A:ILE:H	12	0.61
(2,1228)	1:122:A:ILE:HG22	1:124:A:SER:H	4	0.61
(2,1226)	1:95:A:LEU:HD11	1:95:A:LEU:H	7	0.61
(2,1226)	1:91:A:ILE:HG22	1:95:A:LEU:H	12	0.61
(2,1225)	1:95:A:LEU:HD21	1:95:A:LEU:H	5	0.61
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	6	0.61
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	13	0.61
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	20	0.61
(2,665)	1:115:A:TYR:HE2	1:112:A:LEU:H	15	0.61
(2,610)	1:24:A:ILE:HG22	1:63:A:LEU:H	6	0.61
(2,607)	1:66:A:ILE:HG23	1:64:A:VAL:H	13	0.61
(2,550)	1:24:A:ILE:HG13	1:63:A:LEU:H	4	0.61
(2,550)	1:24:A:ILE:HG13	1:63:A:LEU:H	19	0.61
(2,248)	1:36:A:LEU:HD13	1:36:A:LEU:H	6	0.61
(2,245)	1:44:A:ILE:HD12	1:44:A:ILE:H	2	0.61
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	15	0.61
(2,77)	1:56:A:ILE:HD12	1:61:A:TRP:HE1	10	0.61
(2,77)	1:56:A:ILE:HD11	1:61:A:TRP:HE1	17	0.61
(2,4570)	1:60:A:LEU:HD23	1:86:A:TRP:HD1	9	0.6
(2,4519)	1:119:A:ILE:HG22	1:68:A:PHE:HD2	14	0.6
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD2	14	0.6
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	19	0.6
(2,4351)	1:111:A:LEU:HD23	1:91:A:ILE:HD11	8	0.6
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD13	4	0.6
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD11	6	0.6
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD12	10	0.6
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB3	16	0.6
(2,4210)	1:81:A:VAL:HA	1:91:A:ILE:HD12	2	0.6
(2,4126)	1:79:A:TYR:HA	1:103:A:ILE:HD13	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4105)	1:79:A:TYR:HD1	1:71:A:ILE:HD13	18	0.6
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD12	2	0.6
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD13	4	0.6
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD12	10	0.6
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG23	5	0.6
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	4	0.6
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG11	1	0.6
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD21	9	0.6
(2,3717)	1:61:A:TRP:HZ3	1:28:A:LEU:HD21	20	0.6
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD22	20	0.6
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD21	8	0.6
(2,3703)	1:70:A:PHE:HD2	1:112:A:LEU:HD22	12	0.6
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD21	10	0.6
(2,3635)	1:52:A:LEU:HD12	1:56:A:ILE:HG12	17	0.6
(2,3609)	1:126:A:THR:HG23	1:125:A:PRO:HG2	3	0.6
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG22	5	0.6
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG23	14	0.6
(2,2874)	1:118:A:LEU:HD22	1:48:A:GLU:HG3	20	0.6
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	18	0.6
(2,2364)	1:93:A:ILE:HG21	1:90:A:ALA:HA	1	0.6
(2,2174)	1:99:A:ILE:HD12	1:89:A:LYS:HA	9	0.6
(2,2174)	1:99:A:ILE:HD13	1:89:A:LYS:HA	14	0.6
(2,2174)	1:99:A:ILE:HD11	1:89:A:LYS:HA	16	0.6
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	12	0.6
(2,1896)	1:60:A:LEU:HD12	1:93:A:ILE:HA	7	0.6
(2,1896)	1:60:A:LEU:HD11	1:93:A:ILE:HA	8	0.6
(2,1885)	1:123:A:LEU:HD21	1:125:A:PRO:HA	2	0.6
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	10	0.6
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	12	0.6
(2,1833)	1:51:A:LYS:HB2	1:54:A:SER:HB2	19	0.6
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	4	0.6
(2,1818)	1:80:A:PHE:HB2	1:81:A:VAL:HA	11	0.6
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	15	0.6
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	6	0.6
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	13	0.6
(2,1557)	1:24:A:ILE:HD13	1:61:A:TRP:HE1	1	0.6
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	15	0.6
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	1	0.6
(2,1256)	1:24:A:ILE:HG23	1:54:A:SER:H	20	0.6
(2,1240)	1:112:A:LEU:HD13	1:113:A:ARG:H	5	0.6
(2,1240)	1:112:A:LEU:HD13	1:113:A:ARG:H	14	0.6
(2,1226)	1:95:A:LEU:HD12	1:95:A:LEU:H	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1226)	1:95:A:LEU:HD11	1:95:A:LEU:H	14	0.6
(2,1226)	1:95:A:LEU:HD13	1:95:A:LEU:H	19	0.6
(2,850)	1:139:A:LEU:HD21	1:140:A:GLU:H	10	0.6
(2,760)	1:41:A:TYR:HB2	1:34:A:ILE:H	8	0.6
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	3	0.6
(2,610)	1:24:A:ILE:HG23	1:63:A:LEU:H	10	0.6
(2,610)	1:24:A:ILE:HG21	1:63:A:LEU:H	14	0.6
(2,610)	1:24:A:ILE:HG21	1:63:A:LEU:H	15	0.6
(2,607)	1:66:A:ILE:HG21	1:64:A:VAL:H	19	0.6
(2,596)	1:28:A:LEU:HD13	1:50:A:GLU:H	5	0.6
(2,583)	1:94:A:LEU:HD22	1:55:A:ARG:H	5	0.6
(2,550)	1:24:A:ILE:HG13	1:63:A:LEU:H	3	0.6
(2,550)	1:60:A:LEU:HB2	1:63:A:LEU:H	6	0.6
(2,550)	1:25:A:LYS:HG3	1:63:A:LEU:H	9	0.6
(2,550)	1:60:A:LEU:HB2	1:63:A:LEU:H	13	0.6
(2,333)	1:56:A:ILE:HG22	1:61:A:TRP:H	20	0.6
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	13	0.6
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	15	0.6
(2,248)	1:36:A:LEU:HD12	1:36:A:LEU:H	1	0.6
(2,248)	1:36:A:LEU:HD13	1:36:A:LEU:H	20	0.6
(2,245)	1:32:A:LEU:HD21	1:44:A:ILE:H	15	0.6
(2,235)	1:31:A:LYS:HB3	1:27:A:ALA:H	2	0.6
(2,118)	1:124:A:SER:HB3	1:123:A:LEU:H	20	0.6
(2,116)	1:82:A:SER:HB3	1:120:A:PHE:H	12	0.6
(2,77)	1:56:A:ILE:HD12	1:61:A:TRP:HE1	2	0.6
(2,77)	1:56:A:ILE:HD13	1:61:A:TRP:HE1	5	0.6
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE1	3	0.59
(2,4570)	1:60:A:LEU:HD23	1:86:A:TRP:HD1	3	0.59
(2,4570)	1:60:A:LEU:HD22	1:86:A:TRP:HD1	8	0.59
(2,4474)	1:36:A:LEU:HD22	1:41:A:TYR:HD2	4	0.59
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD11	19	0.59
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG23	11	0.59
(2,4300)	1:65:A:LYS:HE2	1:63:A:LEU:HD22	10	0.59
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD13	4	0.59
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD13	15	0.59
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD13	12	0.59
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD11	13	0.59
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD11	11	0.59
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD13	18	0.59
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD12	5	0.59
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG21	11	0.59
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG23	20	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	2	0.59
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD23	3	0.59
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD21	11	0.59
(2,3280)	1:79:A:TYR:H	1:104:A:LEU:HG	7	0.59
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	3	0.59
(2,2865)	1:76:A:ILE:HG23	1:105:A:ASN:HB2	4	0.59
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	9	0.59
(2,2542)	1:115:A:TYR:HD1	1:111:A:LEU:HB2	9	0.59
(2,2194)	1:58:A:LEU:HD22	1:54:A:SER:HA	13	0.59
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	11	0.59
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	16	0.59
(2,1896)	1:60:A:LEU:HD13	1:93:A:ILE:HA	2	0.59
(2,1896)	1:60:A:LEU:HD13	1:93:A:ILE:HA	12	0.59
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	5	0.59
(2,1866)	1:139:A:LEU:HB2	1:136:A:SER:HB3	13	0.59
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	16	0.59
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	2	0.59
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	4	0.59
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	12	0.59
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	20	0.59
(2,1818)	1:80:A:PHE:HB2	1:81:A:VAL:HA	2	0.59
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	20	0.59
(2,1610)	1:95:A:LEU:HD21	1:110:A:LYS:H	14	0.59
(2,1610)	1:95:A:LEU:HD21	1:110:A:LYS:H	16	0.59
(2,1557)	1:24:A:ILE:HD11	1:61:A:TRP:HE1	11	0.59
(2,1394)	1:64:A:VAL:HG22	1:87:A:ASN:HD22	17	0.59
(2,1256)	1:24:A:ILE:HG21	1:54:A:SER:H	3	0.59
(2,1226)	1:95:A:LEU:HD12	1:95:A:LEU:H	18	0.59
(2,885)	1:66:A:ILE:HD12	1:26:A:ASP:H	5	0.59
(2,863)	1:122:A:ILE:HG21	1:13:A:ILE:H	12	0.59
(2,848)	1:27:A:ALA:HB3	1:26:A:ASP:H	2	0.59
(2,610)	1:24:A:ILE:HG21	1:63:A:LEU:H	1	0.59
(2,607)	1:66:A:ILE:HG22	1:64:A:VAL:H	12	0.59
(2,550)	1:60:A:LEU:HB2	1:63:A:LEU:H	7	0.59
(2,550)	1:24:A:ILE:HG13	1:63:A:LEU:H	18	0.59
(2,331)	1:33:A:LYS:HB3	1:32:A:LEU:H	10	0.59
(2,331)	1:31:A:LYS:HD3	1:32:A:LEU:H	20	0.59
(2,248)	1:36:A:LEU:HD12	1:36:A:LEU:H	14	0.59
(2,248)	1:36:A:LEU:HD11	1:36:A:LEU:H	16	0.59
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	17	0.59
(2,235)	1:25:A:LYS:HB3	1:27:A:ALA:H	18	0.59
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	1	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	5	0.59
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	17	0.59
(2,77)	1:56:A:ILE:HD13	1:61:A:TRP:HE1	3	0.59
(2,4570)	1:60:A:LEU:HD21	1:86:A:TRP:HD1	19	0.58
(2,4551)	1:34:A:ILE:HG23	1:120:A:PHE:HE2	4	0.58
(2,4373)	1:133:A:THR:HG23	1:137:A:GLU:HB3	4	0.58
(2,4351)	1:111:A:LEU:HD21	1:91:A:ILE:HD11	3	0.58
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD12	9	0.58
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB1	9	0.58
(2,4161)	1:89:A:LYS:HE2	1:93:A:ILE:HD12	11	0.58
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD13	2	0.58
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD12	10	0.58
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD12	10	0.58
(2,4107)	1:41:A:TYR:HD1	1:34:A:ILE:HD11	14	0.58
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD13	10	0.58
(2,4093)	1:120:A:PHE:HD1	1:122:A:ILE:HD11	4	0.58
(2,4093)	1:120:A:PHE:HD1	1:69:A:ILE:HD12	7	0.58
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD13	14	0.58
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD12	13	0.58
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG22	7	0.58
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG23	8	0.58
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG23	2	0.58
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG22	8	0.58
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG21	20	0.58
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD21	8	0.58
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG13	4	0.58
(2,3564)	1:55:A:ARG:HD3	1:94:A:LEU:HD12	4	0.58
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	20	0.58
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	5	0.58
(2,3344)	1:119:A:ILE:H	1:119:A:ILE:HG12	9	0.58
(2,3111)	1:22:A:VAL:HA	1:65:A:LYS:HD3	11	0.58
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	6	0.58
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	3	0.58
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	12	0.58
(2,2651)	1:95:A:LEU:HD23	1:110:A:LYS:HE3	20	0.58
(2,2382)	1:103:A:ILE:HG21	1:107:A:ASP:HA	8	0.58
(2,2375)	1:104:A:LEU:HD23	1:78:A:GLU:HA	4	0.58
(2,2375)	1:104:A:LEU:HD21	1:78:A:GLU:HA	7	0.58
(2,2163)	1:102:A:VAL:HG22	1:103:A:ILE:HA	7	0.58
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	20	0.58
(2,1896)	1:60:A:LEU:HD12	1:93:A:ILE:HA	6	0.58
(2,1885)	1:123:A:LEU:HD21	1:125:A:PRO:HA	4	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	9	0.58
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	10	0.58
(2,1847)	1:78:A:GLU:HB3	1:73:A:SER:HB2	20	0.58
(2,1841)	1:89:A:LYS:HG3	1:93:A:ILE:HA	12	0.58
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	3	0.58
(2,1818)	1:80:A:PHE:HB2	1:81:A:VAL:HA	7	0.58
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	7	0.58
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	20	0.58
(2,1497)	1:81:A:VAL:HG11	1:83:A:GLY:H	11	0.58
(2,1330)	1:132:A:GLU:HG2	1:136:A:SER:H	6	0.58
(2,1226)	1:95:A:LEU:HD12	1:95:A:LEU:H	1	0.58
(2,1226)	1:95:A:LEU:HD13	1:95:A:LEU:H	3	0.58
(2,1066)	1:99:A:ILE:HD12	1:97:A:ARG:H	3	0.58
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	5	0.58
(2,760)	1:41:A:TYR:HB2	1:34:A:ILE:H	9	0.58
(2,598)	1:24:A:ILE:HG21	1:52:A:LEU:H	5	0.58
(2,583)	1:94:A:LEU:HD23	1:55:A:ARG:H	2	0.58
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	5	0.58
(2,550)	1:60:A:LEU:HB2	1:63:A:LEU:H	2	0.58
(2,550)	1:60:A:LEU:HB2	1:63:A:LEU:H	15	0.58
(2,550)	1:24:A:ILE:HG13	1:63:A:LEU:H	16	0.58
(2,550)	1:24:A:ILE:HG13	1:63:A:LEU:H	17	0.58
(2,550)	1:60:A:LEU:HB2	1:63:A:LEU:H	20	0.58
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	14	0.58
(2,510)	1:65:A:LYS:HE3	1:64:A:VAL:H	1	0.58
(2,470)	1:53:A:SER:HB3	1:52:A:LEU:H	19	0.58
(2,333)	1:56:A:ILE:HG23	1:61:A:TRP:H	8	0.58
(2,333)	1:56:A:ILE:HG22	1:61:A:TRP:H	14	0.58
(2,248)	1:36:A:LEU:HD13	1:36:A:LEU:H	3	0.58
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	7	0.58
(2,235)	1:25:A:LYS:HB3	1:27:A:ALA:H	4	0.58
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	4	0.58
(2,83)	1:34:A:ILE:HD11	1:43:A:GLU:H	12	0.58
(2,77)	1:56:A:ILE:HD11	1:61:A:TRP:HE1	12	0.58
(2,77)	1:56:A:ILE:HD12	1:61:A:TRP:HE1	16	0.58
(2,77)	1:56:A:ILE:HD13	1:61:A:TRP:HE1	18	0.58
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	14	0.58
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	12	0.58
(2,4570)	1:60:A:LEU:HD23	1:86:A:TRP:HD1	6	0.57
(2,4505)	1:122:A:ILE:HD12	1:14:A:PHE:HD1	2	0.57
(2,4457)	1:20:A:GLU:HG3	1:21:A:TYR:HD1	5	0.57
(2,4438)	1:35:A:ARG:HD3	1:41:A:TYR:HD2	12	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD1	19	0.57
(2,4377)	1:112:A:LEU:HD12	1:109:A:GLU:HG3	15	0.57
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD11	8	0.57
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD11	20	0.57
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD12	2	0.57
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB2	11	0.57
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB1	13	0.57
(2,4300)	1:65:A:LYS:HE2	1:63:A:LEU:HD23	18	0.57
(2,4107)	1:21:A:TYR:HD2	1:34:A:ILE:HD12	12	0.57
(2,4107)	1:41:A:TYR:HD1	1:34:A:ILE:HD12	15	0.57
(2,4092)	1:14:A:PHE:HD1	1:122:A:ILE:HD12	2	0.57
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD11	6	0.57
(2,4091)	1:56:A:ILE:H	1:56:A:ILE:HD11	12	0.57
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD13	1	0.57
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG22	18	0.57
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG23	12	0.57
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG22	3	0.57
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	6	0.57
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG23	3	0.57
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG21	5	0.57
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG11	12	0.57
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG11	18	0.57
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD21	15	0.57
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG23	11	0.57
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD23	16	0.57
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	14	0.57
(2,3361)	1:88:A:LYS:H	1:64:A:VAL:HG22	11	0.57
(2,3344)	1:119:A:ILE:H	1:119:A:ILE:HG12	1	0.57
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD12	1	0.57
(2,3247)	1:60:A:LEU:HD22	1:89:A:LYS:HB3	2	0.57
(2,3072)	1:88:A:LYS:H	1:85:A:GLN:HG2	14	0.57
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	12	0.57
(2,2542)	1:115:A:TYR:HD1	1:111:A:LEU:HB2	3	0.57
(2,2364)	1:93:A:ILE:HG23	1:90:A:ALA:HA	14	0.57
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	16	0.57
(2,1610)	1:95:A:LEU:HD23	1:110:A:LYS:H	1	0.57
(2,1610)	1:95:A:LEU:HD22	1:110:A:LYS:H	13	0.57
(2,1610)	1:95:A:LEU:HD23	1:110:A:LYS:H	19	0.57
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	10	0.57
(2,1257)	1:108:A:VAL:HG12	1:113:A:ARG:H	5	0.57
(2,1256)	1:24:A:ILE:HG21	1:54:A:SER:H	15	0.57
(2,1226)	1:95:A:LEU:HD11	1:95:A:LEU:H	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1219)	1:45:A:LYS:HG3	1:47:A:ASP:H	9	0.57
(2,1036)	1:43:A:GLU:HG2	1:33:A:LYS:H	19	0.57
(2,850)	1:139:A:LEU:HD11	1:140:A:GLU:H	14	0.57
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	11	0.57
(2,610)	1:24:A:ILE:HG23	1:63:A:LEU:H	4	0.57
(2,610)	1:24:A:ILE:HG23	1:63:A:LEU:H	17	0.57
(2,550)	1:60:A:LEU:HB2	1:63:A:LEU:H	10	0.57
(2,470)	1:53:A:SER:HB3	1:52:A:LEU:H	12	0.57
(2,333)	1:56:A:ILE:HG23	1:61:A:TRP:H	3	0.57
(2,333)	1:56:A:ILE:HG21	1:61:A:TRP:H	6	0.57
(2,333)	1:56:A:ILE:HG23	1:61:A:TRP:H	9	0.57
(2,331)	1:33:A:LYS:HB3	1:32:A:LEU:H	1	0.57
(2,245)	1:32:A:LEU:HD23	1:44:A:ILE:H	18	0.57
(2,235)	1:31:A:LYS:HB3	1:27:A:ALA:H	10	0.57
(2,225)	1:98:A:GLU:HG3	1:99:A:ILE:H	3	0.57
(2,166)	1:22:A:VAL:HG11	1:31:A:LYS:H	10	0.57
(2,166)	1:22:A:VAL:HG12	1:31:A:LYS:H	10	0.57
(2,166)	1:22:A:VAL:HG13	1:31:A:LYS:H	10	0.57
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	3	0.57
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	6	0.57
(2,4689)	1:123:A:LEU:HD23	1:79:A:TYR:HD1	15	0.56
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE2	17	0.56
(2,4570)	1:60:A:LEU:HD23	1:86:A:TRP:HD1	10	0.56
(2,4570)	1:60:A:LEU:HD22	1:86:A:TRP:HD1	15	0.56
(2,4469)	1:35:A:ARG:HG3	1:41:A:TYR:HD2	9	0.56
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	1	0.56
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD13	18	0.56
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB3	17	0.56
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG22	14	0.56
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD11	14	0.56
(2,4107)	1:41:A:TYR:HD2	1:34:A:ILE:HD12	5	0.56
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD11	12	0.56
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD12	14	0.56
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD11	18	0.56
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD11	19	0.56
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG22	6	0.56
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG22	9	0.56
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG12	13	0.56
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG11	13	0.56
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG13	19	0.56
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD23	18	0.56
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG22	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG21	7	0.56
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD23	17	0.56
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD23	10	0.56
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD22	15	0.56
(2,3635)	1:52:A:LEU:HD11	1:56:A:ILE:HG12	14	0.56
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	10	0.56
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	6	0.56
(2,3463)	1:87:A:ASN:HA	1:88:A:LYS:HG3	17	0.56
(2,3344)	1:119:A:ILE:H	1:119:A:ILE:HG12	10	0.56
(2,3299)	1:44:A:ILE:H	1:33:A:LYS:HG2	17	0.56
(2,3271)	1:28:A:LEU:HD13	1:25:A:LYS:HD3	2	0.56
(2,3247)	1:60:A:LEU:HD22	1:89:A:LYS:HB3	17	0.56
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	14	0.56
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	10	0.56
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	15	0.56
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	16	0.56
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	1	0.56
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	16	0.56
(2,1557)	1:24:A:ILE:HD12	1:61:A:TRP:HE1	10	0.56
(2,1557)	1:24:A:ILE:HD13	1:61:A:TRP:HE1	20	0.56
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	14	0.56
(2,1501)	1:95:A:LEU:HD11	1:96:A:GLY:H	8	0.56
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	19	0.56
(2,1378)	1:109:A:GLU:HB2	1:105:A:ASN:HD22	7	0.56
(2,1314)	1:100:A:SER:HB3	1:101:A:ASN:HD21	17	0.56
(2,1256)	1:24:A:ILE:HG21	1:54:A:SER:H	18	0.56
(2,1240)	1:112:A:LEU:HD13	1:113:A:ARG:H	8	0.56
(2,1234)	1:94:A:LEU:HD23	1:56:A:ILE:H	9	0.56
(2,1234)	1:94:A:LEU:HD22	1:56:A:ILE:H	10	0.56
(2,1226)	1:95:A:LEU:HD11	1:95:A:LEU:H	8	0.56
(2,1226)	1:95:A:LEU:HD12	1:95:A:LEU:H	16	0.56
(2,1225)	1:95:A:LEU:HD22	1:95:A:LEU:H	14	0.56
(2,760)	1:41:A:TYR:HB2	1:34:A:ILE:H	1	0.56
(2,610)	1:24:A:ILE:HG21	1:63:A:LEU:H	13	0.56
(2,598)	1:24:A:ILE:HG22	1:52:A:LEU:H	16	0.56
(2,583)	1:94:A:LEU:HD23	1:55:A:ARG:H	4	0.56
(2,564)	1:104:A:LEU:HD23	1:79:A:TYR:H	10	0.56
(2,564)	1:104:A:LEU:HD22	1:79:A:TYR:H	15	0.56
(2,550)	1:24:A:ILE:HG13	1:63:A:LEU:H	11	0.56
(2,550)	1:24:A:ILE:HG13	1:63:A:LEU:H	12	0.56
(2,333)	1:56:A:ILE:HG23	1:61:A:TRP:H	18	0.56
(2,248)	1:36:A:LEU:HD12	1:36:A:LEU:H	4	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,245)	1:44:A:ILE:HD12	1:44:A:ILE:H	16	0.56
(2,235)	1:31:A:LYS:HB3	1:27:A:ALA:H	13	0.56
(2,235)	1:25:A:LYS:HB3	1:27:A:ALA:H	17	0.56
(2,116)	1:82:A:SER:HB3	1:120:A:PHE:H	8	0.56
(2,4551)	1:122:A:ILE:HD12	1:120:A:PHE:HE1	14	0.55
(2,4519)	1:119:A:ILE:HG23	1:68:A:PHE:HD2	13	0.55
(2,4519)	1:119:A:ILE:HG23	1:68:A:PHE:HD1	17	0.55
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD1	16	0.55
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD13	3	0.55
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD12	18	0.55
(2,4125)	1:104:A:LEU:HA	1:103:A:ILE:HD13	18	0.55
(2,4120)	1:21:A:TYR:HA	1:34:A:ILE:HD11	2	0.55
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD12	7	0.55
(2,4107)	1:21:A:TYR:HD2	1:34:A:ILE:HD11	2	0.55
(2,4107)	1:41:A:TYR:HD1	1:34:A:ILE:HD13	3	0.55
(2,4107)	1:21:A:TYR:HD2	1:34:A:ILE:HD11	6	0.55
(2,4107)	1:21:A:TYR:HD2	1:34:A:ILE:HD13	17	0.55
(2,4107)	1:41:A:TYR:HD1	1:34:A:ILE:HD11	19	0.55
(2,4105)	1:79:A:TYR:HD2	1:71:A:ILE:HD13	13	0.55
(2,4092)	1:14:A:PHE:HD1	1:122:A:ILE:HD11	15	0.55
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG22	13	0.55
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG23	10	0.55
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG21	2	0.55
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG23	13	0.55
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	9	0.55
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG11	6	0.55
(2,3773)	1:60:A:LEU:HA	1:63:A:LEU:HD22	2	0.55
(2,3705)	1:14:A:PHE:HD1	1:10:A:LEU:HD23	4	0.55
(2,3635)	1:52:A:LEU:HD13	1:56:A:ILE:HG12	9	0.55
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD12	13	0.55
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	9	0.55
(2,3344)	1:70:A:PHE:HD2	1:119:A:ILE:HG12	4	0.55
(2,3344)	1:70:A:PHE:HD1	1:119:A:ILE:HG12	11	0.55
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	1	0.55
(2,2863)	1:22:A:VAL:HG12	1:26:A:ASP:HB3	4	0.55
(2,2863)	1:22:A:VAL:HG13	1:26:A:ASP:HB3	10	0.55
(2,2364)	1:93:A:ILE:HG23	1:90:A:ALA:HA	13	0.55
(2,2194)	1:28:A:LEU:HD12	1:54:A:SER:HA	20	0.55
(2,2175)	1:94:A:LEU:HD22	1:52:A:LEU:HA	11	0.55
(2,2163)	1:102:A:VAL:HG22	1:103:A:ILE:HA	17	0.55
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	8	0.55
(2,2097)	1:93:A:ILE:HG13	1:89:A:LYS:HA	10	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1899)	1:76:A:ILE:HD13	1:73:A:SER:HB3	18	0.55
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	3	0.55
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	19	0.55
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	20	0.55
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	5	0.55
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	11	0.55
(2,1626)	1:135:A:LEU:HD13	1:136:A:SER:H	7	0.55
(2,1501)	1:95:A:LEU:HD11	1:96:A:GLY:H	20	0.55
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	7	0.55
(2,1240)	1:112:A:LEU:HD11	1:113:A:ARG:H	19	0.55
(2,1234)	1:94:A:LEU:HD23	1:56:A:ILE:H	7	0.55
(2,1228)	1:123:A:LEU:HD21	1:124:A:SER:H	2	0.55
(2,1228)	1:123:A:LEU:HD22	1:124:A:SER:H	6	0.55
(2,1066)	1:99:A:ILE:HD11	1:97:A:ARG:H	19	0.55
(2,1036)	1:43:A:GLU:HG2	1:33:A:LYS:H	15	0.55
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	5	0.55
(2,610)	1:24:A:ILE:HG23	1:63:A:LEU:H	2	0.55
(2,610)	1:24:A:ILE:HG23	1:63:A:LEU:H	8	0.55
(2,607)	1:66:A:ILE:HG22	1:64:A:VAL:H	2	0.55
(2,598)	1:24:A:ILE:HG21	1:52:A:LEU:H	8	0.55
(2,564)	1:104:A:LEU:HD13	1:79:A:TYR:H	12	0.55
(2,348)	1:58:A:LEU:HD22	1:61:A:TRP:H	6	0.55
(2,333)	1:56:A:ILE:HG22	1:61:A:TRP:H	4	0.55
(2,333)	1:56:A:ILE:HG22	1:61:A:TRP:H	10	0.55
(2,83)	1:34:A:ILE:HD12	1:43:A:GLU:H	16	0.55
(2,77)	1:56:A:ILE:HD12	1:61:A:TRP:HE1	15	0.55
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	19	0.55
(2,4689)	1:123:A:LEU:HD21	1:79:A:TYR:HD1	3	0.54
(2,4570)	1:60:A:LEU:HD23	1:86:A:TRP:HD1	4	0.54
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD11	11	0.54
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD13	4	0.54
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD12	5	0.54
(2,4276)	1:111:A:LEU:HD23	1:114:A:GLU:HB2	7	0.54
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD13	15	0.54
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD11	17	0.54
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD13	9	0.54
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD13	2	0.54
(2,4093)	1:120:A:PHE:HD2	1:122:A:ILE:HD12	16	0.54
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG23	1	0.54
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG21	20	0.54
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG23	15	0.54
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG22	5	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG23	17	0.54
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB3	15	0.54
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG22	7	0.54
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG12	15	0.54
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG11	16	0.54
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD21	19	0.54
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD21	7	0.54
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD22	8	0.54
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD21	19	0.54
(2,3635)	1:52:A:LEU:HD13	1:56:A:ILE:HG12	8	0.54
(2,3601)	1:56:A:ILE:HB	1:52:A:LEU:HD11	19	0.54
(2,3389)	1:41:A:TYR:HD2	1:36:A:LEU:HG	14	0.54
(2,3344)	1:70:A:PHE:HD2	1:119:A:ILE:HG12	6	0.54
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	5	0.54
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	2	0.54
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	15	0.54
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	20	0.54
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	6	0.54
(2,2364)	1:93:A:ILE:HG22	1:90:A:ALA:HA	17	0.54
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	8	0.54
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	17	0.54
(2,1833)	1:50:A:GLU:HB3	1:54:A:SER:HB2	13	0.54
(2,1818)	1:80:A:PHE:HB2	1:81:A:VAL:HA	8	0.54
(2,1818)	1:80:A:PHE:HB2	1:81:A:VAL:HA	12	0.54
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	20	0.54
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	13	0.54
(2,1499)	1:93:A:ILE:HG21	1:96:A:GLY:H	12	0.54
(2,1499)	1:93:A:ILE:HG22	1:96:A:GLY:H	20	0.54
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	12	0.54
(2,1398)	1:119:A:ILE:HD11	1:114:A:GLU:H	11	0.54
(2,1398)	1:119:A:ILE:HD13	1:114:A:GLU:H	14	0.54
(2,1314)	1:100:A:SER:HB2	1:101:A:ASN:HD21	14	0.54
(2,1255)	1:28:A:LEU:HD21	1:54:A:SER:H	19	0.54
(2,1234)	1:94:A:LEU:HD23	1:56:A:ILE:H	4	0.54
(2,1234)	1:94:A:LEU:HD23	1:56:A:ILE:H	20	0.54
(2,1225)	1:95:A:LEU:HD22	1:95:A:LEU:H	2	0.54
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	10	0.54
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	4	0.54
(2,610)	1:24:A:ILE:HG21	1:63:A:LEU:H	18	0.54
(2,596)	1:28:A:LEU:HD12	1:50:A:GLU:H	4	0.54
(2,316)	1:31:A:LYS:HE3	1:32:A:LEU:H	17	0.54
(2,245)	1:44:A:ILE:HD13	1:44:A:ILE:H	1	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:34:A:ILE:HD13	1:43:A:GLU:H	9	0.54
(2,77)	1:56:A:ILE:HD11	1:61:A:TRP:HE1	11	0.54
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE1	18	0.53
(2,4518)	1:76:A:ILE:HD13	1:80:A:PHE:HZ	15	0.53
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD13	1	0.53
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD12	7	0.53
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD13	8	0.53
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD13	14	0.53
(2,4276)	1:111:A:LEU:HD21	1:114:A:GLU:HB2	5	0.53
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD11	4	0.53
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD11	3	0.53
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD11	5	0.53
(2,4093)	1:120:A:PHE:HD1	1:122:A:ILE:HD11	3	0.53
(2,4065)	1:68:A:PHE:H	1:66:A:ILE:HD11	13	0.53
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG23	4	0.53
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG23	18	0.53
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG21	4	0.53
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG21	7	0.53
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG22	16	0.53
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG23	19	0.53
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG21	12	0.53
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG12	11	0.53
(2,3717)	1:37:A:ASN:HD21	1:36:A:LEU:HD22	9	0.53
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD23	19	0.53
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG22	15	0.53
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD23	16	0.53
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD21	11	0.53
(2,3463)	1:87:A:ASN:HA	1:88:A:LYS:HG3	3	0.53
(2,3435)	1:22:A:VAL:HA	1:65:A:LYS:HG3	6	0.53
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	6	0.53
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	16	0.53
(2,3344)	1:70:A:PHE:HD1	1:119:A:ILE:HG12	16	0.53
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD23	6	0.53
(2,3280)	1:79:A:TYR:H	1:104:A:LEU:HG	17	0.53
(2,3111)	1:79:A:TYR:HA	1:72:A:LYS:HD3	5	0.53
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	8	0.53
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	4	0.53
(2,2842)	1:25:A:LYS:HB2	1:26:A:ASP:HB2	18	0.53
(2,2473)	1:69:A:ILE:HD13	1:18:A:PRO:HD3	1	0.53
(2,2382)	1:103:A:ILE:HG21	1:107:A:ASP:HA	5	0.53
(2,2364)	1:93:A:ILE:HG23	1:90:A:ALA:HA	5	0.53
(2,2338)	1:72:A:LYS:HD3	1:79:A:TYR:HA	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2194)	1:58:A:LEU:HD21	1:54:A:SER:HA	4	0.53
(2,2163)	1:102:A:VAL:HG22	1:103:A:ILE:HA	3	0.53
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	11	0.53
(2,1896)	1:60:A:LEU:HD11	1:93:A:ILE:HA	15	0.53
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	5	0.53
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	17	0.53
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	1	0.53
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	9	0.53
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	18	0.53
(2,1626)	1:135:A:LEU:HD22	1:136:A:SER:H	5	0.53
(2,1501)	1:95:A:LEU:HD12	1:96:A:GLY:H	16	0.53
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	8	0.53
(2,1240)	1:112:A:LEU:HD11	1:113:A:ARG:H	13	0.53
(2,1234)	1:94:A:LEU:HD22	1:56:A:ILE:H	5	0.53
(2,1234)	1:94:A:LEU:HD21	1:56:A:ILE:H	6	0.53
(2,1234)	1:94:A:LEU:HD22	1:56:A:ILE:H	18	0.53
(2,1228)	1:123:A:LEU:HD21	1:124:A:SER:H	8	0.53
(2,1225)	1:95:A:LEU:HD22	1:95:A:LEU:H	7	0.53
(2,1066)	1:99:A:ILE:HD13	1:97:A:ARG:H	9	0.53
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	7	0.53
(2,851)	1:106:A:VAL:HG11	1:108:A:VAL:H	4	0.53
(2,851)	1:106:A:VAL:HG11	1:108:A:VAL:H	15	0.53
(2,841)	1:5:A:ILE:HD12	1:5:A:ILE:H	4	0.53
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	8	0.53
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	9	0.53
(2,610)	1:24:A:ILE:HG21	1:63:A:LEU:H	3	0.53
(2,564)	1:104:A:LEU:HD21	1:79:A:TYR:H	11	0.53
(2,510)	1:65:A:LYS:HE3	1:64:A:VAL:H	5	0.53
(2,333)	1:56:A:ILE:HG23	1:61:A:TRP:H	16	0.53
(2,333)	1:56:A:ILE:HG22	1:61:A:TRP:H	17	0.53
(2,160)	1:71:A:ILE:HG12	1:70:A:PHE:H	17	0.53
(2,156)	1:69:A:ILE:HD13	1:120:A:PHE:H	17	0.53
(2,83)	1:34:A:ILE:HD12	1:43:A:GLU:H	5	0.53
(2,4656)	1:72:A:LYS:HE2	1:79:A:TYR:HE2	9	0.52
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE2	2	0.52
(2,4519)	1:52:A:LEU:HD23	1:68:A:PHE:HD1	15	0.52
(2,4373)	1:133:A:THR:HG22	1:137:A:GLU:HB3	2	0.52
(2,4333)	1:18:A:PRO:HD3	1:122:A:ILE:HD11	5	0.52
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD13	10	0.52
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD13	13	0.52
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD11	16	0.52
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD13	19	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD11	11	0.52
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB1	1	0.52
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB1	18	0.52
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD12	6	0.52
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD13	11	0.52
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD13	1	0.52
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD11	7	0.52
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD13	16	0.52
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD13	9	0.52
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG23	18	0.52
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG21	9	0.52
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG23	15	0.52
(2,3925)	1:21:A:TYR:HE1	1:34:A:ILE:HG21	19	0.52
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG21	3	0.52
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG21	20	0.52
(2,3836)	1:90:A:ALA:HB2	1:64:A:VAL:HG12	14	0.52
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG13	7	0.52
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG11	9	0.52
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG11	12	0.52
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG11	17	0.52
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG13	20	0.52
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG21	4	0.52
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD23	2	0.52
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD22	14	0.52
(2,3609)	1:13:A:ILE:HG13	1:125:A:PRO:HG2	19	0.52
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	3	0.52
(2,3501)	1:112:A:LEU:HA	1:121:A:ILE:HG13	15	0.52
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	20	0.52
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	8	0.52
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD13	6	0.52
(2,3271)	1:28:A:LEU:HD12	1:25:A:LYS:HD3	5	0.52
(2,3247)	1:60:A:LEU:HD23	1:89:A:LYS:HB3	9	0.52
(2,3247)	1:60:A:LEU:HD22	1:89:A:LYS:HB3	15	0.52
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	10	0.52
(2,3072)	1:88:A:LYS:H	1:85:A:GLN:HG2	11	0.52
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	20	0.52
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	11	0.52
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	1	0.52
(2,2874)	1:118:A:LEU:HD23	1:48:A:GLU:HG3	17	0.52
(2,2560)	1:42:A:HIS:HD2	1:34:A:ILE:HB	8	0.52
(2,2473)	1:122:A:ILE:HD11	1:18:A:PRO:HD3	5	0.52
(2,2194)	1:28:A:LEU:HD11	1:54:A:SER:HA	2	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2175)	1:94:A:LEU:HD22	1:52:A:LEU:HA	12	0.52
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	14	0.52
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	18	0.52
(2,2074)	1:25:A:LYS:HE2	1:25:A:LYS:HA	13	0.52
(2,1896)	1:60:A:LEU:HD11	1:93:A:ILE:HA	16	0.52
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	6	0.52
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	15	0.52
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	10	0.52
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	19	0.52
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	6	0.52
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	11	0.52
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	15	0.52
(2,1686)	1:24:A:ILE:HG23	1:23:A:THR:HB	1	0.52
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	1	0.52
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	4	0.52
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	2	0.52
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	8	0.52
(2,1501)	1:95:A:LEU:HD11	1:96:A:GLY:H	2	0.52
(2,1404)	1:122:A:ILE:HD13	1:37:A:ASN:HD22	6	0.52
(2,1378)	1:109:A:GLU:HB2	1:105:A:ASN:HD22	20	0.52
(2,1256)	1:24:A:ILE:HG21	1:54:A:SER:H	9	0.52
(2,1255)	1:52:A:LEU:HD12	1:54:A:SER:H	5	0.52
(2,1236)	1:19:A:ALA:HB1	1:38:A:ASN:H	14	0.52
(2,1228)	1:123:A:LEU:HD21	1:124:A:SER:H	13	0.52
(2,1225)	1:95:A:LEU:HD22	1:95:A:LEU:H	11	0.52
(2,1225)	1:95:A:LEU:HD23	1:95:A:LEU:H	18	0.52
(2,841)	1:139:A:LEU:HD21	1:139:A:LEU:H	20	0.52
(2,610)	1:24:A:ILE:HG21	1:63:A:LEU:H	9	0.52
(2,607)	1:66:A:ILE:HG22	1:64:A:VAL:H	11	0.52
(2,564)	1:104:A:LEU:HD23	1:79:A:TYR:H	2	0.52
(2,564)	1:104:A:LEU:HD22	1:79:A:TYR:H	14	0.52
(2,248)	1:36:A:LEU:HD11	1:36:A:LEU:H	11	0.52
(2,235)	1:31:A:LYS:HB3	1:27:A:ALA:H	7	0.52
(2,166)	1:22:A:VAL:HG11	1:31:A:LYS:H	3	0.52
(2,166)	1:22:A:VAL:HG12	1:31:A:LYS:H	3	0.52
(2,166)	1:22:A:VAL:HG13	1:31:A:LYS:H	3	0.52
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	11	0.52
(2,83)	1:34:A:ILE:HD13	1:43:A:GLU:H	10	0.52
(2,4551)	1:122:A:ILE:HD12	1:120:A:PHE:HE2	5	0.51
(2,4505)	1:122:A:ILE:HD12	1:14:A:PHE:HD2	4	0.51
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD1	13	0.51
(2,4438)	1:35:A:ARG:HD3	1:41:A:TYR:HD1	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4373)	1:133:A:THR:HG22	1:137:A:GLU:HB3	1	0.51
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD13	9	0.51
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD12	15	0.51
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD11	6	0.51
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD13	15	0.51
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD13	7	0.51
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD12	15	0.51
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	10	0.51
(2,4222)	1:71:A:ILE:HB	1:73:A:SER:HB2	4	0.51
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD13	6	0.51
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD12	3	0.51
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD12	2	0.51
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD13	19	0.51
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD12	6	0.51
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD11	17	0.51
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD12	20	0.51
(2,4092)	1:14:A:PHE:HD2	1:122:A:ILE:HD12	4	0.51
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD12	3	0.51
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG23	19	0.51
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG22	5	0.51
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG23	18	0.51
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG21	18	0.51
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG21	1	0.51
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG22	4	0.51
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG22	12	0.51
(2,3836)	1:90:A:ALA:HB1	1:64:A:VAL:HG11	11	0.51
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD21	1	0.51
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG11	19	0.51
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD21	16	0.51
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	15	0.51
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	17	0.51
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD21	10	0.51
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD13	4	0.51
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD13	16	0.51
(2,3299)	1:44:A:ILE:H	1:33:A:LYS:HG2	2	0.51
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	17	0.51
(2,3017)	1:66:A:ILE:H	1:65:A:LYS:HD3	12	0.51
(2,2844)	1:51:A:LYS:HG3	1:47:A:ASP:HB3	9	0.51
(2,2382)	1:28:A:LEU:HD21	1:47:A:ASP:HA	2	0.51
(2,2364)	1:93:A:ILE:HG23	1:90:A:ALA:HA	18	0.51
(2,2194)	1:28:A:LEU:HD13	1:54:A:SER:HA	10	0.51
(2,2194)	1:28:A:LEU:HD11	1:54:A:SER:HA	17	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2163)	1:102:A:VAL:HG23	1:103:A:ILE:HA	14	0.51
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	15	0.51
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	7	0.51
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	2	0.51
(2,1686)	1:24:A:ILE:HG23	1:23:A:THR:HB	14	0.51
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	17	0.51
(2,1610)	1:95:A:LEU:HD21	1:110:A:LYS:H	3	0.51
(2,1501)	1:95:A:LEU:HD11	1:96:A:GLY:H	6	0.51
(2,1389)	1:106:A:VAL:HG12	1:105:A:ASN:HD21	2	0.51
(2,1240)	1:112:A:LEU:HD11	1:113:A:ARG:H	16	0.51
(2,1226)	1:95:A:LEU:HD12	1:95:A:LEU:H	11	0.51
(2,1180)	1:26:A:ASP:HB3	1:22:A:VAL:H	13	0.51
(2,1066)	1:99:A:ILE:HD12	1:97:A:ARG:H	18	0.51
(2,1056)	1:91:A:ILE:HG22	1:92:A:SER:H	12	0.51
(2,1027)	1:90:A:ALA:HB1	1:92:A:SER:H	3	0.51
(2,885)	1:66:A:ILE:HD12	1:26:A:ASP:H	19	0.51
(2,848)	1:27:A:ALA:HB2	1:26:A:ASP:H	20	0.51
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	1	0.51
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	6	0.51
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	8	0.51
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	10	0.51
(2,665)	1:70:A:PHE:HZ	1:112:A:LEU:H	13	0.51
(2,607)	1:66:A:ILE:HG21	1:64:A:VAL:H	7	0.51
(2,564)	1:104:A:LEU:HD21	1:79:A:TYR:H	16	0.51
(2,527)	1:72:A:LYS:HB2	1:79:A:TYR:H	3	0.51
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	20	0.51
(2,510)	1:65:A:LYS:HE2	1:64:A:VAL:H	3	0.51
(2,333)	1:56:A:ILE:HG22	1:61:A:TRP:H	12	0.51
(2,333)	1:56:A:ILE:HG23	1:61:A:TRP:H	15	0.51
(2,333)	1:56:A:ILE:HG23	1:61:A:TRP:H	19	0.51
(2,248)	1:36:A:LEU:HD13	1:36:A:LEU:H	8	0.51
(2,245)	1:44:A:ILE:HD11	1:44:A:ILE:H	14	0.51
(2,166)	1:22:A:VAL:HG11	1:31:A:LYS:H	7	0.51
(2,166)	1:22:A:VAL:HG12	1:31:A:LYS:H	7	0.51
(2,166)	1:22:A:VAL:HG13	1:31:A:LYS:H	7	0.51
(2,77)	1:56:A:ILE:HD13	1:61:A:TRP:HE1	1	0.51
(2,77)	1:56:A:ILE:HD13	1:61:A:TRP:HE1	7	0.51
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	8	0.51
(2,4641)	1:78:A:GLU:HA	1:79:A:TYR:HE2	18	0.5
(2,4551)	1:34:A:ILE:HG22	1:120:A:PHE:HE2	12	0.5
(2,4518)	1:76:A:ILE:HD12	1:80:A:PHE:HZ	2	0.5
(2,4465)	1:118:A:LEU:HD13	1:115:A:TYR:HD2	3	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4457)	1:20:A:GLU:HG3	1:21:A:TYR:HD1	15	0.5
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD2	2	0.5
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD1	13	0.5
(2,4385)	1:129:A:TYR:HB3	1:131:A:GLU:HG3	20	0.5
(2,4374)	1:135:A:LEU:HD21	1:134:A:GLU:HB3	7	0.5
(2,4374)	1:135:A:LEU:HD11	1:131:A:GLU:HB2	15	0.5
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD12	7	0.5
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD12	3	0.5
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD12	11	0.5
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD11	4	0.5
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG21	20	0.5
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG21	12	0.5
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG21	10	0.5
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG23	3	0.5
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG21	20	0.5
(2,3836)	1:90:A:ALA:HB1	1:64:A:VAL:HG13	20	0.5
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG11	3	0.5
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD22	19	0.5
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	6	0.5
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	7	0.5
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	2	0.5
(2,3354)	1:61:A:TRP:HZ3	1:25:A:LYS:HG2	3	0.5
(2,3247)	1:60:A:LEU:HD23	1:89:A:LYS:HB3	10	0.5
(2,3247)	1:60:A:LEU:HD21	1:89:A:LYS:HB3	19	0.5
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	7	0.5
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	9	0.5
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	18	0.5
(2,2376)	1:34:A:ILE:HD13	1:42:A:HIS:HA	12	0.5
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	13	0.5
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	19	0.5
(2,2074)	1:25:A:LYS:HE2	1:25:A:LYS:HA	5	0.5
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	12	0.5
(2,1866)	1:139:A:LEU:HB2	1:136:A:SER:HB3	17	0.5
(2,1808)	1:92:A:SER:HB3	1:91:A:ILE:HA	3	0.5
(2,1781)	1:68:A:PHE:HE1	1:91:A:ILE:HA	12	0.5
(2,1680)	1:125:A:PRO:HB2	1:126:A:THR:HB	12	0.5
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	10	0.5
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	15	0.5
(2,1601)	1:43:A:GLU:HG3	1:34:A:ILE:H	19	0.5
(2,1557)	1:24:A:ILE:HD12	1:61:A:TRP:HE1	8	0.5
(2,1557)	1:24:A:ILE:HD12	1:61:A:TRP:HE1	13	0.5
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	13	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1501)	1:95:A:LEU:HD12	1:96:A:GLY:H	9	0.5
(2,1499)	1:93:A:ILE:HG22	1:96:A:GLY:H	19	0.5
(2,1256)	1:24:A:ILE:HG21	1:54:A:SER:H	13	0.5
(2,1228)	1:123:A:LEU:HD21	1:124:A:SER:H	18	0.5
(2,1225)	1:95:A:LEU:HD22	1:95:A:LEU:H	3	0.5
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	2	0.5
(2,885)	1:66:A:ILE:HD12	1:26:A:ASP:H	13	0.5
(2,850)	1:22:A:VAL:HG21	1:26:A:ASP:H	19	0.5
(2,848)	1:27:A:ALA:HB3	1:26:A:ASP:H	10	0.5
(2,607)	1:66:A:ILE:HG23	1:64:A:VAL:H	18	0.5
(2,598)	1:24:A:ILE:HG22	1:52:A:LEU:H	13	0.5
(2,333)	1:56:A:ILE:HG23	1:61:A:TRP:H	13	0.5
(2,316)	1:31:A:LYS:HE2	1:32:A:LEU:H	3	0.5
(2,245)	1:44:A:ILE:HD11	1:44:A:ILE:H	3	0.5
(2,100)	1:79:A:TYR:HE1	1:70:A:PHE:H	1	0.5
(2,4667)	1:94:A:LEU:HD22	1:115:A:TYR:HE2	17	0.49
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE2	7	0.49
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD1	5	0.49
(2,4334)	1:120:A:PHE:HB2	1:122:A:ILE:HD12	14	0.49
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD13	4	0.49
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD13	2	0.49
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD12	11	0.49
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD11	20	0.49
(2,4243)	1:102:A:VAL:HG21	1:104:A:LEU:HA	8	0.49
(2,4222)	1:71:A:ILE:HB	1:73:A:SER:HB2	14	0.49
(2,4107)	1:41:A:TYR:HD1	1:34:A:ILE:HD13	13	0.49
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD13	4	0.49
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG23	8	0.49
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG21	17	0.49
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG21	3	0.49
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG23	6	0.49
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG22	12	0.49
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG12	4	0.49
(2,3705)	1:14:A:PHE:HD1	1:10:A:LEU:HD23	10	0.49
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD23	19	0.49
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD21	9	0.49
(2,3670)	1:103:A:ILE:H	1:104:A:LEU:HD22	12	0.49
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	10	0.49
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	18	0.49
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD12	5	0.49
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD22	3	0.49
(2,3111)	1:22:A:VAL:HA	1:65:A:LYS:HD3	13	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	3	0.49
(2,2542)	1:115:A:TYR:HD1	1:111:A:LEU:HB2	1	0.49
(2,2542)	1:115:A:TYR:HD1	1:111:A:LEU:HB2	8	0.49
(2,2542)	1:115:A:TYR:HD2	1:111:A:LEU:HB2	11	0.49
(2,2473)	1:69:A:ILE:HD13	1:18:A:PRO:HD3	4	0.49
(2,2338)	1:65:A:LYS:HD2	1:21:A:TYR:HA	6	0.49
(2,2175)	1:94:A:LEU:HD22	1:52:A:LEU:HA	5	0.49
(2,2081)	1:43:A:GLU:HG3	1:41:A:TYR:HA	1	0.49
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	14	0.49
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	12	0.49
(2,1833)	1:51:A:LYS:HB2	1:54:A:SER:HB2	14	0.49
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	3	0.49
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	5	0.49
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	14	0.49
(2,1626)	1:139:A:LEU:HD13	1:136:A:SER:H	11	0.49
(2,1610)	1:95:A:LEU:HD21	1:110:A:LYS:H	10	0.49
(2,1550)	1:48:A:GLU:HG2	1:46:A:LYS:H	9	0.49
(2,1248)	1:94:A:LEU:HD13	1:95:A:LEU:H	1	0.49
(2,1240)	1:112:A:LEU:HD11	1:113:A:ARG:H	1	0.49
(2,1234)	1:94:A:LEU:HD23	1:56:A:ILE:H	17	0.49
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	14	0.49
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	18	0.49
(2,1019)	1:67:A:PRO:HB3	1:66:A:ILE:H	20	0.49
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	20	0.49
(2,877)	1:60:A:LEU:HD22	1:86:A:TRP:H	8	0.49
(2,868)	1:23:A:THR:HG21	1:24:A:ILE:H	7	0.49
(2,868)	1:23:A:THR:HG21	1:24:A:ILE:H	14	0.49
(2,851)	1:106:A:VAL:HG13	1:108:A:VAL:H	10	0.49
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	18	0.49
(2,760)	1:41:A:TYR:HB2	1:34:A:ILE:H	11	0.49
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	5	0.49
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	12	0.49
(2,610)	1:24:A:ILE:HG21	1:63:A:LEU:H	11	0.49
(2,607)	1:66:A:ILE:HG23	1:64:A:VAL:H	14	0.49
(2,333)	1:56:A:ILE:HG23	1:61:A:TRP:H	5	0.49
(2,333)	1:56:A:ILE:HG22	1:61:A:TRP:H	7	0.49
(2,333)	1:56:A:ILE:HG23	1:61:A:TRP:H	11	0.49
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	19	0.49
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	1	0.49
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	16	0.49
(2,235)	1:25:A:LYS:HB3	1:27:A:ALA:H	1	0.49
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	14	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	18	0.49
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE2	8	0.48
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE1	10	0.48
(2,4519)	1:119:A:ILE:HG23	1:68:A:PHE:HD2	8	0.48
(2,4519)	1:119:A:ILE:HG22	1:68:A:PHE:HD2	19	0.48
(2,4505)	1:122:A:ILE:HG23	1:14:A:PHE:HD2	9	0.48
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE2	9	0.48
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD1	4	0.48
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD1	19	0.48
(2,4457)	1:43:A:GLU:HG3	1:41:A:TYR:HD2	7	0.48
(2,4351)	1:111:A:LEU:HD22	1:91:A:ILE:HD11	5	0.48
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD11	14	0.48
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB1	8	0.48
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB2	10	0.48
(2,4276)	1:111:A:LEU:HD23	1:114:A:GLU:HB2	19	0.48
(2,4254)	1:46:A:LYS:HG2	1:47:A:ASP:HB3	12	0.48
(2,4243)	1:102:A:VAL:HG21	1:104:A:LEU:HA	6	0.48
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	1	0.48
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD11	1	0.48
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD12	2	0.48
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD11	10	0.48
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD12	5	0.48
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD13	8	0.48
(2,4046)	1:24:A:ILE:HD12	1:66:A:ILE:HG22	9	0.48
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG23	13	0.48
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG21	19	0.48
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG21	9	0.48
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG21	20	0.48
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG22	18	0.48
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG23	14	0.48
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG23	15	0.48
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG23	12	0.48
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG23	18	0.48
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG23	13	0.48
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD23	15	0.48
(2,3705)	1:14:A:PHE:HD2	1:10:A:LEU:HD23	12	0.48
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG22	14	0.48
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD22	1	0.48
(2,3635)	1:52:A:LEU:HD11	1:56:A:ILE:HG12	18	0.48
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	16	0.48
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD13	12	0.48
(2,3247)	1:60:A:LEU:HD22	1:89:A:LYS:HB3	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	10	0.48
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	16	0.48
(2,2560)	1:120:A:PHE:HE2	1:34:A:ILE:HB	18	0.48
(2,2538)	1:115:A:TYR:HD2	1:118:A:LEU:HB3	1	0.48
(2,2382)	1:103:A:ILE:HG22	1:107:A:ASP:HA	16	0.48
(2,2175)	1:94:A:LEU:HD23	1:52:A:LEU:HA	1	0.48
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	3	0.48
(2,2074)	1:25:A:LYS:HE2	1:25:A:LYS:HA	16	0.48
(2,1866)	1:139:A:LEU:HB2	1:136:A:SER:HB2	2	0.48
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	9	0.48
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	5	0.48
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	19	0.48
(2,1686)	1:24:A:ILE:HG23	1:23:A:THR:HB	3	0.48
(2,1686)	1:24:A:ILE:HG21	1:23:A:THR:HB	6	0.48
(2,1686)	1:24:A:ILE:HG23	1:23:A:THR:HB	9	0.48
(2,1686)	1:24:A:ILE:HG22	1:23:A:THR:HB	17	0.48
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	19	0.48
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	1	0.48
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	3	0.48
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	7	0.48
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	8	0.48
(2,1435)	1:31:A:LYS:HB3	1:23:A:THR:H	11	0.48
(2,1409)	1:66:A:ILE:HG22	1:87:A:ASN:HD21	15	0.48
(2,1256)	1:28:A:LEU:HD13	1:54:A:SER:H	10	0.48
(2,1234)	1:94:A:LEU:HD22	1:56:A:ILE:H	14	0.48
(2,1226)	1:95:A:LEU:HD12	1:95:A:LEU:H	9	0.48
(2,1180)	1:26:A:ASP:HB3	1:22:A:VAL:H	15	0.48
(2,1066)	1:99:A:ILE:HD11	1:97:A:ARG:H	20	0.48
(2,1027)	1:90:A:ALA:HB3	1:92:A:SER:H	4	0.48
(2,1027)	1:90:A:ALA:HB3	1:92:A:SER:H	10	0.48
(2,885)	1:66:A:ILE:HD11	1:26:A:ASP:H	8	0.48
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	13	0.48
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	7	0.48
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	18	0.48
(2,607)	1:66:A:ILE:HG21	1:64:A:VAL:H	4	0.48
(2,598)	1:24:A:ILE:HG23	1:52:A:LEU:H	19	0.48
(2,583)	1:94:A:LEU:HD22	1:55:A:ARG:H	12	0.48
(2,583)	1:94:A:LEU:HD21	1:55:A:ARG:H	15	0.48
(2,564)	1:104:A:LEU:HD22	1:79:A:TYR:H	1	0.48
(2,396)	1:68:A:PHE:HZ	1:68:A:PHE:H	12	0.48
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	2	0.48
(2,235)	1:25:A:LYS:HB3	1:27:A:ALA:H	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	20	0.48
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	20	0.48
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	20	0.48
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	2	0.48
(2,77)	1:56:A:ILE:HD12	1:61:A:TRP:HE1	19	0.48
(2,33)	1:46:A:LYS:HD3	1:46:A:LYS:H	11	0.48
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	11	0.48
(2,4696)	1:140:A:GLU:HB3	1:142:A:HIS:HD2	4	0.47
(2,4570)	1:60:A:LEU:HD21	1:86:A:TRP:HD1	1	0.47
(2,4570)	1:60:A:LEU:HD23	1:86:A:TRP:HD1	20	0.47
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD1	15	0.47
(2,4385)	1:129:A:TYR:HB3	1:131:A:GLU:HG3	1	0.47
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD11	5	0.47
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD11	6	0.47
(2,4334)	1:120:A:PHE:HB2	1:122:A:ILE:HD12	17	0.47
(2,4333)	1:18:A:PRO:HD3	1:122:A:ILE:HD12	18	0.47
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD11	9	0.47
(2,4325)	1:61:A:TRP:H	1:56:A:ILE:HD12	20	0.47
(2,4310)	1:120:A:PHE:HD2	1:69:A:ILE:HG21	10	0.47
(2,4243)	1:102:A:VAL:HG23	1:104:A:LEU:HA	13	0.47
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD13	6	0.47
(2,4120)	1:21:A:TYR:HA	1:34:A:ILE:HD12	12	0.47
(2,4046)	1:24:A:ILE:HD13	1:66:A:ILE:HG22	11	0.47
(2,4046)	1:24:A:ILE:HD12	1:66:A:ILE:HG22	12	0.47
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG23	1	0.47
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG23	9	0.47
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG21	12	0.47
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG21	4	0.47
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG22	17	0.47
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG21	12	0.47
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG12	16	0.47
(2,3703)	1:70:A:PHE:HD2	1:112:A:LEU:HD21	18	0.47
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG22	9	0.47
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD23	5	0.47
(2,3635)	1:52:A:LEU:HD12	1:56:A:ILE:HG12	15	0.47
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD22	8	0.47
(2,3501)	1:112:A:LEU:HA	1:121:A:ILE:HG13	17	0.47
(2,3361)	1:87:A:ASN:HD22	1:64:A:VAL:HG21	20	0.47
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	13	0.47
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD21	4	0.47
(2,3247)	1:60:A:LEU:HD21	1:89:A:LYS:HB3	13	0.47
(2,3201)	1:115:A:TYR:HB2	1:114:A:GLU:HB2	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3072)	1:88:A:LYS:H	1:85:A:GLN:HG2	12	0.47
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	18	0.47
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	13	0.47
(2,3050)	1:142:A:HIS:HD2	1:142:A:HIS:HB3	13	0.47
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	16	0.47
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	20	0.47
(2,2874)	1:118:A:LEU:HD21	1:48:A:GLU:HG3	19	0.47
(2,2863)	1:22:A:VAL:HG11	1:26:A:ASP:HB3	7	0.47
(2,2496)	1:32:A:LEU:HB2	1:30:A:GLY:HA2	13	0.47
(2,2473)	1:122:A:ILE:HD12	1:18:A:PRO:HD3	18	0.47
(2,2194)	1:58:A:LEU:HD23	1:54:A:SER:HA	16	0.47
(2,2175)	1:94:A:LEU:HD21	1:52:A:LEU:HA	6	0.47
(2,2163)	1:102:A:VAL:HG23	1:103:A:ILE:HA	2	0.47
(2,2163)	1:102:A:VAL:HG21	1:103:A:ILE:HA	11	0.47
(2,2163)	1:102:A:VAL:HG23	1:103:A:ILE:HA	15	0.47
(2,2143)	1:130:A:THR:HG21	1:131:A:GLU:HA	9	0.47
(2,2074)	1:25:A:LYS:HE2	1:25:A:LYS:HA	7	0.47
(2,1899)	1:76:A:ILE:HD13	1:73:A:SER:HB3	4	0.47
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	8	0.47
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	17	0.47
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	20	0.47
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	13	0.47
(2,1714)	1:131:A:GLU:HB3	1:130:A:THR:HB	7	0.47
(2,1686)	1:24:A:ILE:HG23	1:23:A:THR:HB	11	0.47
(2,1626)	1:135:A:LEU:HD21	1:136:A:SER:H	10	0.47
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	15	0.47
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	4	0.47
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	17	0.47
(2,1557)	1:24:A:ILE:HD13	1:61:A:TRP:HE1	16	0.47
(2,1228)	1:123:A:LEU:HD22	1:124:A:SER:H	5	0.47
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	5	0.47
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	11	0.47
(2,1066)	1:99:A:ILE:HD12	1:97:A:ARG:H	15	0.47
(2,885)	1:66:A:ILE:HD12	1:26:A:ASP:H	9	0.47
(2,877)	1:60:A:LEU:HD21	1:86:A:TRP:H	19	0.47
(2,874)	1:49:A:VAL:HG22	1:48:A:GLU:H	7	0.47
(2,868)	1:23:A:THR:HG22	1:24:A:ILE:H	1	0.47
(2,868)	1:23:A:THR:HG22	1:24:A:ILE:H	16	0.47
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	14	0.47
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	20	0.47
(2,610)	1:24:A:ILE:HG21	1:63:A:LEU:H	16	0.47
(2,607)	1:66:A:ILE:HG23	1:64:A:VAL:H	20	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,598)	1:24:A:ILE:HG21	1:52:A:LEU:H	10	0.47
(2,583)	1:94:A:LEU:HD22	1:55:A:ARG:H	14	0.47
(2,560)	1:95:A:LEU:HD11	1:104:A:LEU:H	11	0.47
(2,396)	1:68:A:PHE:HZ	1:68:A:PHE:H	1	0.47
(2,396)	1:68:A:PHE:HZ	1:68:A:PHE:H	4	0.47
(2,348)	1:58:A:LEU:HD22	1:61:A:TRP:H	14	0.47
(2,333)	1:56:A:ILE:HG22	1:61:A:TRP:H	2	0.47
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	18	0.47
(2,83)	1:34:A:ILE:HD12	1:43:A:GLU:H	6	0.47
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	1	0.47
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	5	0.47
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE1	13	0.46
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE2	13	0.46
(2,4697)	1:146:A:HIS:HB3	1:146:A:HIS:HD2	7	0.46
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE1	1	0.46
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE1	12	0.46
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE2	13	0.46
(2,4570)	1:60:A:LEU:HD21	1:86:A:TRP:HD1	14	0.46
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD2	17	0.46
(2,4374)	1:135:A:LEU:HD22	1:134:A:GLU:HB3	13	0.46
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD12	6	0.46
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD13	14	0.46
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD13	16	0.46
(2,4331)	1:61:A:TRP:HB2	1:24:A:ILE:HD13	19	0.46
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD13	3	0.46
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB3	3	0.46
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG22	1	0.46
(2,4276)	1:111:A:LEU:HD21	1:114:A:GLU:HB2	2	0.46
(2,4243)	1:102:A:VAL:HG23	1:104:A:LEU:HA	5	0.46
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	11	0.46
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD11	9	0.46
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD12	16	0.46
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD11	14	0.46
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD11	6	0.46
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG22	2	0.46
(2,4046)	1:24:A:ILE:HD13	1:66:A:ILE:HG22	5	0.46
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG21	15	0.46
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG22	16	0.46
(2,3927)	1:42:A:HIS:HD2	1:44:A:ILE:HG23	15	0.46
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB1	19	0.46
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB2	3	0.46
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG22	16	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3881)	1:65:A:LYS:H	1:90:A:ALA:HB3	6	0.46
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG22	11	0.46
(2,3836)	1:90:A:ALA:HB3	1:64:A:VAL:HG12	2	0.46
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG11	12	0.46
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG13	5	0.46
(2,3799)	1:107:A:ASP:HB3	1:95:A:LEU:HD22	13	0.46
(2,3794)	1:124:A:SER:HB3	1:126:A:THR:HG22	8	0.46
(2,3703)	1:70:A:PHE:HD2	1:112:A:LEU:HD23	7	0.46
(2,3685)	1:27:A:ALA:H	1:49:A:VAL:HG23	2	0.46
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD21	6	0.46
(2,3635)	1:52:A:LEU:HD12	1:56:A:ILE:HG12	11	0.46
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD22	2	0.46
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD23	20	0.46
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	12	0.46
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	19	0.46
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD11	6	0.46
(2,3247)	1:60:A:LEU:HD21	1:89:A:LYS:HB3	1	0.46
(2,3247)	1:60:A:LEU:HD22	1:89:A:LYS:HB3	18	0.46
(2,3201)	1:115:A:TYR:HB2	1:114:A:GLU:HB2	20	0.46
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	8	0.46
(2,2560)	1:42:A:HIS:HD2	1:34:A:ILE:HB	10	0.46
(2,2542)	1:115:A:TYR:HD2	1:111:A:LEU:HB2	6	0.46
(2,2473)	1:69:A:ILE:HD12	1:18:A:PRO:HD3	6	0.46
(2,2473)	1:69:A:ILE:HD13	1:18:A:PRO:HD3	14	0.46
(2,2473)	1:69:A:ILE:HD13	1:18:A:PRO:HD3	16	0.46
(2,2375)	1:118:A:LEU:HD12	1:115:A:TYR:HA	17	0.46
(2,2174)	1:99:A:ILE:HD11	1:89:A:LYS:HA	18	0.46
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	2	0.46
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	7	0.46
(2,1877)	1:137:A:GLU:HB2	1:136:A:SER:HB2	18	0.46
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	16	0.46
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	14	0.46
(2,1847)	1:78:A:GLU:HB3	1:73:A:SER:HB2	19	0.46
(2,1686)	1:24:A:ILE:HG23	1:23:A:THR:HB	15	0.46
(2,1686)	1:24:A:ILE:HG23	1:23:A:THR:HB	18	0.46
(2,1677)	1:65:A:LYS:HE2	1:23:A:THR:HB	18	0.46
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	9	0.46
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	5	0.46
(2,1610)	1:95:A:LEU:HD22	1:110:A:LYS:H	18	0.46
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	13	0.46
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	7	0.46
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	16	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1499)	1:93:A:ILE:HG22	1:96:A:GLY:H	11	0.46
(2,1256)	1:24:A:ILE:HG23	1:54:A:SER:H	4	0.46
(2,1234)	1:94:A:LEU:HD23	1:56:A:ILE:H	1	0.46
(2,1234)	1:94:A:LEU:HD22	1:56:A:ILE:H	19	0.46
(2,1225)	1:95:A:LEU:HD23	1:95:A:LEU:H	13	0.46
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	19	0.46
(2,1056)	1:91:A:ILE:HG22	1:92:A:SER:H	19	0.46
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	15	0.46
(2,885)	1:66:A:ILE:HD11	1:26:A:ASP:H	1	0.46
(2,868)	1:23:A:THR:HG22	1:24:A:ILE:H	4	0.46
(2,868)	1:23:A:THR:HG21	1:24:A:ILE:H	12	0.46
(2,868)	1:23:A:THR:HG23	1:24:A:ILE:H	18	0.46
(2,864)	1:111:A:LEU:HD12	1:111:A:LEU:H	19	0.46
(2,851)	1:106:A:VAL:HG13	1:108:A:VAL:H	5	0.46
(2,851)	1:106:A:VAL:HG12	1:108:A:VAL:H	12	0.46
(2,851)	1:106:A:VAL:HG11	1:108:A:VAL:H	19	0.46
(2,841)	1:139:A:LEU:HD21	1:139:A:LEU:H	10	0.46
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	12	0.46
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	3	0.46
(2,610)	1:24:A:ILE:HG21	1:63:A:LEU:H	12	0.46
(2,598)	1:24:A:ILE:HG21	1:52:A:LEU:H	20	0.46
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	9	0.46
(2,396)	1:68:A:PHE:HZ	1:68:A:PHE:H	13	0.46
(2,396)	1:68:A:PHE:HZ	1:68:A:PHE:H	18	0.46
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	4	0.46
(2,83)	1:34:A:ILE:HD12	1:43:A:GLU:H	1	0.46
(2,83)	1:34:A:ILE:HD13	1:43:A:GLU:H	2	0.46
(2,77)	1:56:A:ILE:HD12	1:61:A:TRP:HE1	9	0.46
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	13	0.46
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	17	0.46
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	20	0.46
(2,33)	1:46:A:LYS:HD3	1:46:A:LYS:H	9	0.46
(2,4689)	1:123:A:LEU:HD22	1:79:A:TYR:HD1	11	0.45
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE2	8	0.45
(2,4518)	1:76:A:ILE:HD13	1:80:A:PHE:HZ	13	0.45
(2,4383)	1:18:A:PRO:HG2	1:67:A:PRO:HB2	17	0.45
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD13	4	0.45
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD12	14	0.45
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG21	15	0.45
(2,4243)	1:102:A:VAL:HG23	1:104:A:LEU:HA	14	0.45
(2,4243)	1:102:A:VAL:HG22	1:104:A:LEU:HA	17	0.45
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4207)	1:70:A:PHE:HE2	1:91:A:ILE:HD13	17	0.45
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD13	8	0.45
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD12	8	0.45
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG23	3	0.45
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG23	12	0.45
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG21	3	0.45
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG22	6	0.45
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG22	7	0.45
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD23	17	0.45
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG23	5	0.45
(2,3681)	1:129:A:TYR:H	1:126:A:THR:HG23	2	0.45
(2,3676)	1:34:A:ILE:H	1:36:A:LEU:HD21	2	0.45
(2,3361)	1:87:A:ASN:HD22	1:64:A:VAL:HG22	13	0.45
(2,3344)	1:70:A:PHE:HD2	1:119:A:ILE:HG12	2	0.45
(2,3344)	1:70:A:PHE:HD2	1:119:A:ILE:HG12	12	0.45
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	15	0.45
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD21	2	0.45
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD23	17	0.45
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	14	0.45
(2,2874)	1:118:A:LEU:HD21	1:48:A:GLU:HG3	10	0.45
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	13	0.45
(2,2560)	1:21:A:TYR:HE1	1:34:A:ILE:HB	1	0.45
(2,2560)	1:42:A:HIS:HD2	1:34:A:ILE:HB	2	0.45
(2,2560)	1:42:A:HIS:HD2	1:34:A:ILE:HB	4	0.45
(2,2490)	1:31:A:LYS:HG3	1:30:A:GLY:HA3	13	0.45
(2,2364)	1:93:A:ILE:HG23	1:90:A:ALA:HA	4	0.45
(2,2364)	1:93:A:ILE:HG22	1:90:A:ALA:HA	9	0.45
(2,2194)	1:28:A:LEU:HD13	1:54:A:SER:HA	9	0.45
(2,2175)	1:94:A:LEU:HD23	1:52:A:LEU:HA	4	0.45
(2,2174)	1:99:A:ILE:HD11	1:89:A:LYS:HA	8	0.45
(2,2143)	1:130:A:THR:HG21	1:131:A:GLU:HA	1	0.45
(2,2143)	1:133:A:THR:HG21	1:134:A:GLU:HA	20	0.45
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	16	0.45
(2,1990)	1:14:A:PHE:HD1	1:11:A:LYS:HA	16	0.45
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	1	0.45
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	11	0.45
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	13	0.45
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	18	0.45
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	20	0.45
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	18	0.45
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	13	0.45
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	19	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	18	0.45
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	7	0.45
(2,1808)	1:92:A:SER:HB3	1:91:A:ILE:HA	14	0.45
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	18	0.45
(2,1686)	1:24:A:ILE:HG22	1:23:A:THR:HB	7	0.45
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	12	0.45
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	13	0.45
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	16	0.45
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	19	0.45
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	12	0.45
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	17	0.45
(2,1541)	1:22:A:VAL:HB	1:30:A:GLY:H	4	0.45
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	20	0.45
(2,1256)	1:28:A:LEU:HD11	1:54:A:SER:H	17	0.45
(2,1240)	1:112:A:LEU:HD11	1:113:A:ARG:H	11	0.45
(2,1240)	1:112:A:LEU:HD13	1:113:A:ARG:H	12	0.45
(2,1236)	1:19:A:ALA:HB1	1:38:A:ASN:H	5	0.45
(2,1226)	1:95:A:LEU:HD11	1:95:A:LEU:H	2	0.45
(2,1226)	1:95:A:LEU:HD11	1:95:A:LEU:H	6	0.45
(2,1225)	1:95:A:LEU:HD23	1:95:A:LEU:H	15	0.45
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	4	0.45
(2,1180)	1:26:A:ASP:HB3	1:22:A:VAL:H	4	0.45
(2,1180)	1:45:A:LYS:HE2	1:47:A:ASP:H	11	0.45
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	3	0.45
(2,1104)	1:37:A:ASN:H	1:20:A:GLU:H	20	0.45
(2,1019)	1:67:A:PRO:HB3	1:66:A:ILE:H	7	0.45
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	2	0.45
(2,877)	1:60:A:LEU:HD23	1:86:A:TRP:H	9	0.45
(2,868)	1:23:A:THR:HG22	1:24:A:ILE:H	17	0.45
(2,851)	1:106:A:VAL:HG12	1:108:A:VAL:H	7	0.45
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	19	0.45
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	4	0.45
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	4	0.45
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	7	0.45
(2,607)	1:66:A:ILE:HG22	1:64:A:VAL:H	16	0.45
(2,607)	1:66:A:ILE:HG21	1:64:A:VAL:H	17	0.45
(2,598)	1:24:A:ILE:HG21	1:52:A:LEU:H	7	0.45
(2,598)	1:24:A:ILE:HG22	1:52:A:LEU:H	15	0.45
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	10	0.45
(2,527)	1:72:A:LYS:HB2	1:79:A:TYR:H	19	0.45
(2,396)	1:68:A:PHE:HZ	1:68:A:PHE:H	16	0.45
(2,245)	1:44:A:ILE:HD13	1:44:A:ILE:H	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,225)	1:98:A:GLU:HG2	1:99:A:ILE:H	6	0.45
(2,83)	1:34:A:ILE:HD13	1:43:A:GLU:H	8	0.45
(2,83)	1:34:A:ILE:HD12	1:43:A:GLU:H	11	0.45
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	14	0.45
(2,4697)	1:142:A:HIS:HB2	1:142:A:HIS:HD2	12	0.44
(2,4667)	1:111:A:LEU:HD21	1:115:A:TYR:HE1	8	0.44
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE2	6	0.44
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	7	0.44
(2,4570)	1:60:A:LEU:HD22	1:86:A:TRP:HD1	18	0.44
(2,4519)	1:119:A:ILE:HG21	1:68:A:PHE:HD1	7	0.44
(2,4505)	1:122:A:ILE:HG22	1:14:A:PHE:HD2	17	0.44
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	3	0.44
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE2	8	0.44
(2,4474)	1:36:A:LEU:HD21	1:41:A:TYR:HD1	20	0.44
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD2	4	0.44
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD2	9	0.44
(2,4377)	1:112:A:LEU:HD13	1:109:A:GLU:HG3	4	0.44
(2,4373)	1:133:A:THR:HG22	1:137:A:GLU:HB3	11	0.44
(2,4373)	1:133:A:THR:HG21	1:137:A:GLU:HB3	16	0.44
(2,4373)	1:130:A:THR:HG23	1:134:A:GLU:HB3	17	0.44
(2,4351)	1:111:A:LEU:HD21	1:91:A:ILE:HD12	16	0.44
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB3	1	0.44
(2,4310)	1:120:A:PHE:HD2	1:69:A:ILE:HG21	9	0.44
(2,4276)	1:111:A:LEU:HD21	1:114:A:GLU:HB2	8	0.44
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	6	0.44
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	16	0.44
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB3	5	0.44
(2,4211)	1:88:A:LYS:HA	1:91:A:ILE:HD12	13	0.44
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD12	11	0.44
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD11	4	0.44
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD12	13	0.44
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG23	12	0.44
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD12	16	0.44
(2,4093)	1:120:A:PHE:HD1	1:122:A:ILE:HD12	14	0.44
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG21	5	0.44
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG21	13	0.44
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG23	8	0.44
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG23	4	0.44
(2,3836)	1:90:A:ALA:HB2	1:64:A:VAL:HG12	16	0.44
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD22	7	0.44
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD21	19	0.44
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD22	15	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3501)	1:112:A:LEU:HA	1:121:A:ILE:HG13	16	0.44
(2,3471)	1:118:A:LEU:HA	1:44:A:ILE:HG12	9	0.44
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	4	0.44
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	9	0.44
(2,3435)	1:22:A:VAL:HA	1:65:A:LYS:HG3	7	0.44
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	10	0.44
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD11	17	0.44
(2,3271)	1:58:A:LEU:HD22	1:25:A:LYS:HD3	14	0.44
(2,3247)	1:60:A:LEU:HD21	1:89:A:LYS:HB3	12	0.44
(2,3085)	1:21:A:TYR:HD2	1:20:A:GLU:HB2	15	0.44
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	16	0.44
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	6	0.44
(2,3038)	1:90:A:ALA:H	1:89:A:LYS:HD2	10	0.44
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	20	0.44
(2,2874)	1:118:A:LEU:HD22	1:48:A:GLU:HG3	7	0.44
(2,2874)	1:118:A:LEU:HD21	1:48:A:GLU:HG3	15	0.44
(2,2863)	1:22:A:VAL:HG13	1:26:A:ASP:HB3	5	0.44
(2,2658)	1:81:A:VAL:HG22	1:79:A:TYR:HB2	9	0.44
(2,2538)	1:115:A:TYR:HD1	1:118:A:LEU:HB3	7	0.44
(2,2496)	1:46:A:LYS:HG3	1:30:A:GLY:HA2	3	0.44
(2,2364)	1:93:A:ILE:HG23	1:90:A:ALA:HA	11	0.44
(2,2194)	1:58:A:LEU:HD21	1:54:A:SER:HA	18	0.44
(2,2174)	1:99:A:ILE:HD13	1:89:A:LYS:HA	20	0.44
(2,1899)	1:76:A:ILE:HG23	1:73:A:SER:HB2	10	0.44
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	4	0.44
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	16	0.44
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	2	0.44
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	3	0.44
(2,1874)	1:69:A:ILE:HG13	1:82:A:SER:HB3	12	0.44
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	13	0.44
(2,1808)	1:92:A:SER:HB3	1:91:A:ILE:HA	16	0.44
(2,1632)	1:138:A:MET:HB3	1:136:A:SER:H	4	0.44
(2,1626)	1:135:A:LEU:HD21	1:136:A:SER:H	12	0.44
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	2	0.44
(2,1610)	1:95:A:LEU:HD21	1:110:A:LYS:H	2	0.44
(2,1557)	1:24:A:ILE:HD13	1:61:A:TRP:HE1	12	0.44
(2,1486)	1:69:A:ILE:HG13	1:83:A:GLY:H	9	0.44
(2,1240)	1:112:A:LEU:HD12	1:113:A:ARG:H	6	0.44
(2,1240)	1:112:A:LEU:HD12	1:113:A:ARG:H	15	0.44
(2,1234)	1:94:A:LEU:HD22	1:56:A:ILE:H	11	0.44
(2,1234)	1:94:A:LEU:HD21	1:56:A:ILE:H	15	0.44
(2,1056)	1:91:A:ILE:HG21	1:92:A:SER:H	15	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,868)	1:23:A:THR:HG22	1:24:A:ILE:H	3	0.44
(2,868)	1:23:A:THR:HG21	1:24:A:ILE:H	6	0.44
(2,868)	1:23:A:THR:HG21	1:24:A:ILE:H	9	0.44
(2,868)	1:23:A:THR:HG23	1:24:A:ILE:H	10	0.44
(2,868)	1:23:A:THR:HG23	1:24:A:ILE:H	15	0.44
(2,868)	1:23:A:THR:HG21	1:24:A:ILE:H	20	0.44
(2,864)	1:111:A:LEU:HD13	1:111:A:LEU:H	11	0.44
(2,864)	1:111:A:LEU:HD13	1:111:A:LEU:H	14	0.44
(2,851)	1:106:A:VAL:HG12	1:108:A:VAL:H	13	0.44
(2,850)	1:139:A:LEU:HD11	1:140:A:GLU:H	1	0.44
(2,848)	1:27:A:ALA:HB3	1:26:A:ASP:H	19	0.44
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	19	0.44
(2,663)	1:115:A:TYR:HD1	1:112:A:LEU:H	1	0.44
(2,607)	1:66:A:ILE:HG23	1:64:A:VAL:H	3	0.44
(2,605)	1:28:A:LEU:HD23	1:51:A:LYS:H	15	0.44
(2,598)	1:24:A:ILE:HG22	1:52:A:LEU:H	11	0.44
(2,583)	1:94:A:LEU:HD23	1:55:A:ARG:H	1	0.44
(2,564)	1:104:A:LEU:HD23	1:79:A:TYR:H	4	0.44
(2,564)	1:104:A:LEU:HD21	1:79:A:TYR:H	19	0.44
(2,396)	1:68:A:PHE:HZ	1:68:A:PHE:H	5	0.44
(2,396)	1:120:A:PHE:HE1	1:68:A:PHE:H	15	0.44
(2,160)	1:121:A:ILE:HG23	1:70:A:PHE:H	14	0.44
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	10	0.44
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	19	0.44
(2,83)	1:34:A:ILE:HD11	1:43:A:GLU:H	7	0.44
(2,83)	1:34:A:ILE:HD11	1:43:A:GLU:H	18	0.44
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	12	0.44
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	4	0.44
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	16	0.44
(2,4669)	1:18:A:PRO:HG3	1:21:A:TYR:HE2	9	0.43
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE1	1	0.43
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	10	0.43
(2,4512)	1:121:A:ILE:HD12	1:79:A:TYR:HD2	13	0.43
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD1	18	0.43
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD2	17	0.43
(2,4377)	1:135:A:LEU:HD22	1:134:A:GLU:HG3	19	0.43
(2,4373)	1:130:A:THR:HG23	1:134:A:GLU:HB3	14	0.43
(2,4373)	1:130:A:THR:HG21	1:134:A:GLU:HB3	15	0.43
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD13	17	0.43
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB1	11	0.43
(2,4300)	1:65:A:LYS:HE3	1:63:A:LEU:HD22	15	0.43
(2,4276)	1:111:A:LEU:HD21	1:114:A:GLU:HB2	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4276)	1:111:A:LEU:HD23	1:114:A:GLU:HB2	16	0.43
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	1	0.43
(2,4249)	1:52:A:LEU:HD13	1:55:A:ARG:HD3	13	0.43
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	2	0.43
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	3	0.43
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD13	7	0.43
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD13	19	0.43
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	11	0.43
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	11	0.43
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	11	0.43
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD11	18	0.43
(2,4120)	1:21:A:TYR:HA	1:34:A:ILE:HD11	6	0.43
(2,4105)	1:79:A:TYR:HD1	1:71:A:ILE:HD12	15	0.43
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD12	3	0.43
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD12	16	0.43
(2,4020)	1:49:A:VAL:HB	1:44:A:ILE:HG22	12	0.43
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG21	2	0.43
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG23	2	0.43
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG23	7	0.43
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	4	0.43
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	4	0.43
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	4	0.43
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	17	0.43
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	17	0.43
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	17	0.43
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG12	18	0.43
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD22	15	0.43
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD22	19	0.43
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG23	10	0.43
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG22	13	0.43
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG22	16	0.43
(2,3564)	1:55:A:ARG:HD3	1:94:A:LEU:HD12	1	0.43
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	8	0.43
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	13	0.43
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD23	12	0.43
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD22	20	0.43
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD11	13	0.43
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD12	18	0.43
(2,3299)	1:44:A:ILE:H	1:33:A:LYS:HG2	3	0.43
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	18	0.43
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	5	0.43
(2,2865)	1:104:A:LEU:HD22	1:105:A:ASN:HB3	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2651)	1:95:A:LEU:HD21	1:110:A:LYS:HE3	17	0.43
(2,2560)	1:120:A:PHE:HE2	1:34:A:ILE:HB	13	0.43
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	6	0.43
(2,2375)	1:104:A:LEU:HD22	1:78:A:GLU:HA	13	0.43
(2,2364)	1:93:A:ILE:HG23	1:90:A:ALA:HA	3	0.43
(2,2175)	1:94:A:LEU:HD23	1:52:A:LEU:HA	13	0.43
(2,2175)	1:94:A:LEU:HD23	1:52:A:LEU:HA	15	0.43
(2,2174)	1:99:A:ILE:HD12	1:89:A:LYS:HA	17	0.43
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	12	0.43
(2,2074)	1:25:A:LYS:HE3	1:25:A:LYS:HA	2	0.43
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	15	0.43
(2,1904)	1:56:A:ILE:HD13	1:53:A:SER:HA	1	0.43
(2,1904)	1:56:A:ILE:HD12	1:53:A:SER:HA	15	0.43
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	3	0.43
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	15	0.43
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	15	0.43
(2,1847)	1:78:A:GLU:HB3	1:73:A:SER:HB2	7	0.43
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	5	0.43
(2,1787)	1:21:A:TYR:HE1	1:17:A:SER:HB3	10	0.43
(2,1677)	1:65:A:LYS:HE2	1:23:A:THR:HB	9	0.43
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	14	0.43
(2,1626)	1:135:A:LEU:HD21	1:136:A:SER:H	18	0.43
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	9	0.43
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	10	0.43
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	11	0.43
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	6	0.43
(2,1541)	1:22:A:VAL:HB	1:30:A:GLY:H	6	0.43
(2,1378)	1:106:A:VAL:HB	1:105:A:ASN:HD22	15	0.43
(2,1256)	1:28:A:LEU:HD11	1:54:A:SER:H	2	0.43
(2,1240)	1:112:A:LEU:HD13	1:113:A:ARG:H	2	0.43
(2,1236)	1:36:A:LEU:HD13	1:38:A:ASN:H	7	0.43
(2,1234)	1:94:A:LEU:HD22	1:56:A:ILE:H	8	0.43
(2,1228)	1:123:A:LEU:HD21	1:124:A:SER:H	10	0.43
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	2	0.43
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	5	0.43
(2,1027)	1:90:A:ALA:HB1	1:92:A:SER:H	16	0.43
(2,895)	1:91:A:ILE:HD13	1:88:A:LYS:H	1	0.43
(2,882)	1:28:A:LEU:HD22	1:28:A:LEU:H	19	0.43
(2,877)	1:60:A:LEU:HD23	1:86:A:TRP:H	6	0.43
(2,868)	1:23:A:THR:HG21	1:24:A:ILE:H	5	0.43
(2,868)	1:23:A:THR:HG22	1:24:A:ILE:H	8	0.43
(2,868)	1:23:A:THR:HG23	1:24:A:ILE:H	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,851)	1:106:A:VAL:HG13	1:108:A:VAL:H	20	0.43
(2,850)	1:22:A:VAL:HG21	1:26:A:ASP:H	9	0.43
(2,850)	1:139:A:LEU:HD21	1:140:A:GLU:H	12	0.43
(2,831)	1:112:A:LEU:HD11	1:112:A:LEU:H	16	0.43
(2,816)	1:51:A:LYS:HG3	1:49:A:VAL:H	9	0.43
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	4	0.43
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	9	0.43
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	16	0.43
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	10	0.43
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	13	0.43
(2,663)	1:115:A:TYR:HD2	1:112:A:LEU:H	11	0.43
(2,396)	1:68:A:PHE:HZ	1:68:A:PHE:H	17	0.43
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	3	0.43
(2,156)	1:69:A:ILE:HD12	1:120:A:PHE:H	15	0.43
(2,77)	1:56:A:ILE:HD12	1:61:A:TRP:HE1	20	0.43
(2,4689)	1:123:A:LEU:HD23	1:79:A:TYR:HD1	2	0.42
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE2	14	0.42
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE1	19	0.42
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE2	14	0.42
(2,4519)	1:52:A:LEU:HD23	1:68:A:PHE:HD1	20	0.42
(2,4474)	1:36:A:LEU:HD21	1:41:A:TYR:HD1	10	0.42
(2,4469)	1:69:A:ILE:HD13	1:21:A:TYR:HD1	19	0.42
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD2	7	0.42
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD1	9	0.42
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD2	11	0.42
(2,4381)	1:130:A:THR:HG22	1:131:A:GLU:HG2	7	0.42
(2,4373)	1:133:A:THR:HG22	1:137:A:GLU:HB3	18	0.42
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD12	1	0.42
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD12	2	0.42
(2,4264)	1:51:A:LYS:HE2	1:114:A:GLU:HG2	15	0.42
(2,4236)	1:118:A:LEU:HD22	1:117:A:SER:HA	8	0.42
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB2	13	0.42
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD11	12	0.42
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD13	10	0.42
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD12	20	0.42
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD13	16	0.42
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD13	7	0.42
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG23	3	0.42
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG21	6	0.42
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG23	10	0.42
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG21	11	0.42
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB1	20	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG21	9	0.42
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG21	2	0.42
(2,3836)	1:90:A:ALA:HB1	1:64:A:VAL:HG11	7	0.42
(2,3744)	1:79:A:TYR:HA	1:102:A:VAL:HG13	2	0.42
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG12	13	0.42
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG23	3	0.42
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD23	3	0.42
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD22	13	0.42
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD22	4	0.42
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD11	10	0.42
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD12	15	0.42
(2,3347)	1:120:A:PHE:HD1	1:69:A:ILE:HG12	19	0.42
(2,3344)	1:70:A:PHE:HD1	1:119:A:ILE:HG12	5	0.42
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	1	0.42
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD11	5	0.42
(2,3201)	1:115:A:TYR:HB2	1:114:A:GLU:HB2	15	0.42
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	18	0.42
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	9	0.42
(2,3053)	1:61:A:TRP:HZ3	1:61:A:TRP:HB3	5	0.42
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	9	0.42
(2,3038)	1:90:A:ALA:H	1:89:A:LYS:HD2	13	0.42
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	12	0.42
(2,2865)	1:76:A:ILE:HG23	1:105:A:ASN:HB2	17	0.42
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	20	0.42
(2,2538)	1:115:A:TYR:HD1	1:118:A:LEU:HB3	3	0.42
(2,2473)	1:69:A:ILE:HD12	1:18:A:PRO:HD3	2	0.42
(2,2175)	1:94:A:LEU:HD22	1:52:A:LEU:HA	3	0.42
(2,2143)	1:133:A:THR:HG21	1:134:A:GLU:HA	5	0.42
(2,1998)	1:115:A:TYR:HD1	1:112:A:LEU:HA	13	0.42
(2,1899)	1:76:A:ILE:HD13	1:73:A:SER:HB3	6	0.42
(2,1879)	1:56:A:ILE:HG13	1:53:A:SER:HA	17	0.42
(2,1877)	1:137:A:GLU:HB2	1:136:A:SER:HB2	1	0.42
(2,1677)	1:65:A:LYS:HE3	1:23:A:THR:HB	14	0.42
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	3	0.42
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	17	0.42
(2,1509)	1:63:A:LEU:HA	1:62:A:SER:H	3	0.42
(2,1499)	1:93:A:ILE:HG22	1:96:A:GLY:H	14	0.42
(2,1435)	1:31:A:LYS:HB3	1:23:A:THR:H	19	0.42
(2,1388)	1:22:A:VAL:HG12	1:21:A:TYR:H	20	0.42
(2,1234)	1:94:A:LEU:HD22	1:56:A:ILE:H	16	0.42
(2,1180)	1:26:A:ASP:HB3	1:22:A:VAL:H	19	0.42
(2,1063)	1:23:A:THR:HG21	1:25:A:LYS:H	11	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1063)	1:23:A:THR:HG21	1:25:A:LYS:H	15	0.42
(2,962)	1:95:A:LEU:HA	1:97:A:ARG:H	8	0.42
(2,882)	1:28:A:LEU:HD23	1:28:A:LEU:H	20	0.42
(2,868)	1:23:A:THR:HG23	1:24:A:ILE:H	13	0.42
(2,864)	1:111:A:LEU:HD11	1:111:A:LEU:H	1	0.42
(2,864)	1:111:A:LEU:HD12	1:111:A:LEU:H	6	0.42
(2,864)	1:111:A:LEU:HD11	1:111:A:LEU:H	18	0.42
(2,851)	1:106:A:VAL:HG11	1:108:A:VAL:H	17	0.42
(2,848)	1:27:A:ALA:HB2	1:26:A:ASP:H	3	0.42
(2,848)	1:27:A:ALA:HB2	1:26:A:ASP:H	7	0.42
(2,663)	1:115:A:TYR:HD1	1:112:A:LEU:H	3	0.42
(2,598)	1:24:A:ILE:HG22	1:52:A:LEU:H	1	0.42
(2,583)	1:94:A:LEU:HD23	1:55:A:ARG:H	20	0.42
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	2	0.42
(2,564)	1:104:A:LEU:HD23	1:79:A:TYR:H	3	0.42
(2,564)	1:104:A:LEU:HD22	1:79:A:TYR:H	6	0.42
(2,564)	1:104:A:LEU:HD22	1:79:A:TYR:H	13	0.42
(2,516)	1:72:A:LYS:HD2	1:80:A:PHE:H	7	0.42
(2,510)	1:65:A:LYS:HE2	1:64:A:VAL:H	18	0.42
(2,396)	1:68:A:PHE:HZ	1:68:A:PHE:H	3	0.42
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	6	0.42
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	17	0.42
(2,245)	1:44:A:ILE:HD11	1:44:A:ILE:H	7	0.42
(2,245)	1:44:A:ILE:HD12	1:44:A:ILE:H	20	0.42
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	16	0.42
(2,83)	1:34:A:ILE:HD13	1:43:A:GLU:H	13	0.42
(2,83)	1:34:A:ILE:HD11	1:43:A:GLU:H	19	0.42
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	20	0.42
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	9	0.42
(2,4570)	1:60:A:LEU:HD21	1:86:A:TRP:HD1	12	0.41
(2,4519)	1:119:A:ILE:HG23	1:68:A:PHE:HD1	5	0.41
(2,4459)	1:33:A:LYS:HB3	1:41:A:TYR:HD1	10	0.41
(2,4385)	1:129:A:TYR:HB3	1:131:A:GLU:HG3	15	0.41
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD11	6	0.41
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD11	17	0.41
(2,4243)	1:102:A:VAL:HG22	1:104:A:LEU:HA	10	0.41
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	14	0.41
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB2	10	0.41
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD13	4	0.41
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD12	5	0.41
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD12	9	0.41
(2,4161)	1:89:A:LYS:HE2	1:93:A:ILE:HD13	16	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD13	3	0.41
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD13	13	0.41
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG22	15	0.41
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG21	16	0.41
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG21	20	0.41
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG21	8	0.41
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG23	18	0.41
(2,3836)	1:90:A:ALA:HB3	1:64:A:VAL:HG13	18	0.41
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	18	0.41
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	18	0.41
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	18	0.41
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD22	17	0.41
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG11	19	0.41
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG23	17	0.41
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG22	20	0.41
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG11	8	0.41
(2,3609)	1:126:A:THR:HG23	1:125:A:PRO:HG2	18	0.41
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	7	0.41
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD11	2	0.41
(2,3344)	1:70:A:PHE:HD1	1:119:A:ILE:HG12	20	0.41
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	11	0.41
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	18	0.41
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD12	11	0.41
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	4	0.41
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	13	0.41
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	5	0.41
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	19	0.41
(2,2874)	1:118:A:LEU:HD22	1:48:A:GLU:HG3	3	0.41
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	17	0.41
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	13	0.41
(2,2653)	1:95:A:LEU:HD12	1:107:A:ASP:HB2	6	0.41
(2,2653)	1:95:A:LEU:HD13	1:107:A:ASP:HB2	7	0.41
(2,2542)	1:115:A:TYR:HD1	1:111:A:LEU:HB2	16	0.41
(2,2490)	1:31:A:LYS:HG2	1:30:A:GLY:HA3	2	0.41
(2,2364)	1:93:A:ILE:HG22	1:90:A:ALA:HA	10	0.41
(2,2143)	1:133:A:THR:HG22	1:134:A:GLU:HA	12	0.41
(2,2081)	1:43:A:GLU:HG3	1:41:A:TYR:HA	4	0.41
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	5	0.41
(2,2081)	1:43:A:GLU:HG3	1:41:A:TYR:HA	6	0.41
(2,2074)	1:61:A:TRP:HB2	1:25:A:LYS:HA	15	0.41
(2,1990)	1:68:A:PHE:HD1	1:66:A:ILE:HA	18	0.41
(2,1904)	1:56:A:ILE:HD11	1:53:A:SER:HA	12	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	14	0.41
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	20	0.41
(2,1866)	1:24:A:ILE:HG13	1:64:A:VAL:HA	6	0.41
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	14	0.41
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	15	0.41
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	16	0.41
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	18	0.41
(2,1808)	1:92:A:SER:HB3	1:91:A:ILE:HA	10	0.41
(2,1686)	1:66:A:ILE:HG21	1:23:A:THR:HB	4	0.41
(2,1686)	1:24:A:ILE:HG22	1:23:A:THR:HB	5	0.41
(2,1686)	1:24:A:ILE:HG22	1:23:A:THR:HB	10	0.41
(2,1686)	1:24:A:ILE:HG23	1:23:A:THR:HB	12	0.41
(2,1686)	1:24:A:ILE:HG23	1:23:A:THR:HB	16	0.41
(2,1680)	1:125:A:PRO:HB2	1:126:A:THR:HB	17	0.41
(2,1660)	1:130:A:THR:HG22	1:132:A:GLU:H	16	0.41
(2,1626)	1:139:A:LEU:HD11	1:136:A:SER:H	19	0.41
(2,1610)	1:95:A:LEU:HD23	1:110:A:LYS:H	5	0.41
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	1	0.41
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	3	0.41
(2,1557)	1:24:A:ILE:HD13	1:61:A:TRP:HE1	9	0.41
(2,1499)	1:93:A:ILE:HG22	1:96:A:GLY:H	13	0.41
(2,1445)	1:65:A:LYS:HG2	1:23:A:THR:H	2	0.41
(2,1248)	1:94:A:LEU:HD12	1:95:A:LEU:H	12	0.41
(2,1248)	1:94:A:LEU:HD12	1:95:A:LEU:H	20	0.41
(2,1240)	1:112:A:LEU:HD11	1:113:A:ARG:H	10	0.41
(2,1228)	1:123:A:LEU:HD21	1:124:A:SER:H	17	0.41
(2,1222)	1:33:A:LYS:HD3	1:41:A:TYR:H	7	0.41
(2,1180)	1:45:A:LYS:HE3	1:47:A:ASP:H	18	0.41
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	4	0.41
(2,1056)	1:91:A:ILE:HG23	1:92:A:SER:H	4	0.41
(2,1056)	1:91:A:ILE:HG22	1:92:A:SER:H	7	0.41
(2,1036)	1:43:A:GLU:HG2	1:33:A:LYS:H	5	0.41
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	10	0.41
(2,895)	1:91:A:ILE:HD11	1:88:A:LYS:H	17	0.41
(2,885)	1:66:A:ILE:HD12	1:26:A:ASP:H	3	0.41
(2,882)	1:28:A:LEU:HD23	1:28:A:LEU:H	10	0.41
(2,882)	1:28:A:LEU:HD23	1:28:A:LEU:H	17	0.41
(2,874)	1:49:A:VAL:HG22	1:48:A:GLU:H	8	0.41
(2,864)	1:111:A:LEU:HD11	1:111:A:LEU:H	7	0.41
(2,864)	1:111:A:LEU:HD11	1:111:A:LEU:H	8	0.41
(2,851)	1:106:A:VAL:HG11	1:108:A:VAL:H	3	0.41
(2,851)	1:106:A:VAL:HG11	1:108:A:VAL:H	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,850)	1:22:A:VAL:HG22	1:26:A:ASP:H	4	0.41
(2,848)	1:27:A:ALA:HB3	1:26:A:ASP:H	12	0.41
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	15	0.41
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	17	0.41
(2,665)	1:115:A:TYR:HE2	1:112:A:LEU:H	19	0.41
(2,663)	1:115:A:TYR:HD1	1:112:A:LEU:H	9	0.41
(2,583)	1:94:A:LEU:HD22	1:55:A:ARG:H	18	0.41
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	5	0.41
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	14	0.41
(2,527)	1:72:A:LYS:HB2	1:79:A:TYR:H	1	0.41
(2,235)	1:25:A:LYS:HB3	1:27:A:ALA:H	12	0.41
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	9	0.41
(2,83)	1:34:A:ILE:HD12	1:43:A:GLU:H	15	0.41
(2,33)	1:46:A:LYS:HD2	1:46:A:LYS:H	10	0.41
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE2	7	0.4
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE2	9	0.4
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	18	0.4
(2,4519)	1:119:A:ILE:HG21	1:68:A:PHE:HD1	10	0.4
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	11	0.4
(2,4374)	1:135:A:LEU:HD11	1:131:A:GLU:HB2	14	0.4
(2,4373)	1:130:A:THR:HG21	1:134:A:GLU:HB3	3	0.4
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD13	18	0.4
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD11	20	0.4
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD11	2	0.4
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD11	3	0.4
(2,4334)	1:120:A:PHE:HB2	1:122:A:ILE:HD12	15	0.4
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD13	18	0.4
(2,4310)	1:120:A:PHE:HD2	1:69:A:ILE:HG23	16	0.4
(2,4276)	1:111:A:LEU:HD21	1:114:A:GLU:HB2	20	0.4
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	4	0.4
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	5	0.4
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	9	0.4
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	19	0.4
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD11	6	0.4
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD13	10	0.4
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD11	18	0.4
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD11	11	0.4
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD11	9	0.4
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD12	9	0.4
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD13	9	0.4
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD11	19	0.4
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD12	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD13	19	0.4
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD13	3	0.4
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD13	6	0.4
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD11	8	0.4
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD11	1	0.4
(2,4120)	1:21:A:TYR:HA	1:34:A:ILE:HD12	8	0.4
(2,4107)	1:41:A:TYR:HD1	1:34:A:ILE:HD12	11	0.4
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD11	1	0.4
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD12	14	0.4
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD13	12	0.4
(2,4046)	1:24:A:ILE:HD12	1:66:A:ILE:HG21	1	0.4
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG22	11	0.4
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG21	11	0.4
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG23	19	0.4
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG21	18	0.4
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG22	2	0.4
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB2	16	0.4
(2,3801)	1:26:A:ASP:HB2	1:22:A:VAL:HG12	8	0.4
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG23	8	0.4
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	19	0.4
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	19	0.4
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	19	0.4
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG12	6	0.4
(2,3635)	1:52:A:LEU:HD13	1:56:A:ILE:HG12	3	0.4
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD21	6	0.4
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	5	0.4
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	13	0.4
(2,3344)	1:70:A:PHE:HD1	1:119:A:ILE:HG12	3	0.4
(2,3344)	1:70:A:PHE:HD2	1:119:A:ILE:HG12	19	0.4
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD21	8	0.4
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD21	13	0.4
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD13	2	0.4
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	19	0.4
(2,3050)	1:142:A:HIS:HD2	1:142:A:HIS:HB3	1	0.4
(2,3050)	1:142:A:HIS:HD2	1:142:A:HIS:HB3	15	0.4
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	3	0.4
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	17	0.4
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	19	0.4
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	9	0.4
(2,2496)	1:46:A:LYS:HG3	1:30:A:GLY:HA2	6	0.4
(2,2163)	1:102:A:VAL:HG21	1:103:A:ILE:HA	8	0.4
(2,1990)	1:68:A:PHE:HD2	1:66:A:ILE:HA	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1948)	1:92:A:SER:H	1:99:A:ILE:HA	8	0.4
(2,1904)	1:56:A:ILE:HD13	1:53:A:SER:HA	3	0.4
(2,1877)	1:90:A:ALA:HB3	1:64:A:VAL:HA	19	0.4
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	19	0.4
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	9	0.4
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	10	0.4
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	19	0.4
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	20	0.4
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	6	0.4
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	12	0.4
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	7	0.4
(2,1627)	1:135:A:LEU:HD11	1:133:A:THR:H	6	0.4
(2,1627)	1:135:A:LEU:HD12	1:133:A:THR:H	6	0.4
(2,1627)	1:135:A:LEU:HD13	1:133:A:THR:H	6	0.4
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	20	0.4
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	14	0.4
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	20	0.4
(2,1256)	1:28:A:LEU:HD13	1:54:A:SER:H	16	0.4
(2,1240)	1:112:A:LEU:HD13	1:113:A:ARG:H	9	0.4
(2,1240)	1:112:A:LEU:HD12	1:113:A:ARG:H	18	0.4
(2,1236)	1:19:A:ALA:HB3	1:38:A:ASN:H	18	0.4
(2,1228)	1:123:A:LEU:HD23	1:124:A:SER:H	7	0.4
(2,1225)	1:95:A:LEU:HD21	1:95:A:LEU:H	19	0.4
(2,1220)	1:99:A:ILE:HG13	1:101:A:ASN:H	8	0.4
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	7	0.4
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	14	0.4
(2,1066)	1:99:A:ILE:HD13	1:97:A:ARG:H	13	0.4
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	2	0.4
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	13	0.4
(2,874)	1:49:A:VAL:HG21	1:48:A:GLU:H	11	0.4
(2,874)	1:49:A:VAL:HG21	1:48:A:GLU:H	17	0.4
(2,874)	1:49:A:VAL:HG22	1:48:A:GLU:H	19	0.4
(2,868)	1:23:A:THR:HG22	1:24:A:ILE:H	19	0.4
(2,864)	1:111:A:LEU:HD11	1:111:A:LEU:H	2	0.4
(2,864)	1:111:A:LEU:HD11	1:111:A:LEU:H	5	0.4
(2,864)	1:111:A:LEU:HD11	1:111:A:LEU:H	15	0.4
(2,850)	1:139:A:LEU:HD13	1:140:A:GLU:H	11	0.4
(2,850)	1:139:A:LEU:HD13	1:140:A:GLU:H	20	0.4
(2,841)	1:139:A:LEU:HD23	1:139:A:LEU:H	13	0.4
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	3	0.4
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	2	0.4
(2,665)	1:115:A:TYR:HE2	1:112:A:LEU:H	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,598)	1:24:A:ILE:HG22	1:52:A:LEU:H	14	0.4
(2,598)	1:24:A:ILE:HG21	1:52:A:LEU:H	17	0.4
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	15	0.4
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	16	0.4
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	17	0.4
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	3	0.4
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	4	0.4
(2,527)	1:72:A:LYS:HB2	1:79:A:TYR:H	6	0.4
(2,245)	1:44:A:ILE:HD11	1:44:A:ILE:H	11	0.4
(2,237)	1:89:A:LYS:HG3	1:93:A:ILE:H	12	0.4
(2,166)	1:22:A:VAL:HG11	1:31:A:LYS:H	4	0.4
(2,166)	1:22:A:VAL:HG12	1:31:A:LYS:H	4	0.4
(2,166)	1:22:A:VAL:HG13	1:31:A:LYS:H	4	0.4
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	13	0.4
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	13	0.4
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	13	0.4
(2,156)	1:69:A:ILE:HD11	1:120:A:PHE:H	13	0.4
(2,154)	1:71:A:ILE:HD12	1:122:A:ILE:H	7	0.4
(2,83)	1:34:A:ILE:HD13	1:43:A:GLU:H	20	0.4
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	6	0.4
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	17	0.4
(2,33)	1:46:A:LYS:HD2	1:46:A:LYS:H	6	0.4
(2,33)	1:46:A:LYS:HD2	1:46:A:LYS:H	17	0.4
(2,4689)	1:123:A:LEU:HD21	1:79:A:TYR:HD1	1	0.39
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE2	4	0.39
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	16	0.39
(2,4570)	1:60:A:LEU:HD22	1:86:A:TRP:HD1	17	0.39
(2,4551)	1:122:A:ILE:HD12	1:120:A:PHE:HE2	15	0.39
(2,4519)	1:119:A:ILE:HG22	1:68:A:PHE:HD1	16	0.39
(2,4465)	1:118:A:LEU:HD12	1:115:A:TYR:HD1	7	0.39
(2,4374)	1:135:A:LEU:HD22	1:134:A:GLU:HB3	3	0.39
(2,4373)	1:130:A:THR:HG22	1:131:A:GLU:HB3	19	0.39
(2,4300)	1:65:A:LYS:HE3	1:63:A:LEU:HD23	17	0.39
(2,4276)	1:111:A:LEU:HD21	1:114:A:GLU:HB2	4	0.39
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD13	18	0.39
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD11	15	0.39
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD11	1	0.39
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD12	1	0.39
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD13	1	0.39
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD12	4	0.39
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD11	5	0.39
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD11	11	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4064)	1:70:A:PHE:H	1:122:A:ILE:HD13	6	0.39
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG23	18	0.39
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG23	17	0.39
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG22	1	0.39
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG23	2	0.39
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG21	13	0.39
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB2	8	0.39
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG22	11	0.39
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG23	4	0.39
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	1	0.39
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	1	0.39
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	1	0.39
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD22	13	0.39
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD22	11	0.39
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD23	8	0.39
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG22	18	0.39
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG13	2	0.39
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG13	12	0.39
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD22	13	0.39
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD13	1	0.39
(2,3389)	1:41:A:TYR:HD2	1:36:A:LEU:HG	4	0.39
(2,3344)	1:70:A:PHE:HD2	1:119:A:ILE:HG12	7	0.39
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	16	0.39
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD12	3	0.39
(2,3111)	1:79:A:TYR:HA	1:72:A:LYS:HD3	14	0.39
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	3	0.39
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	2	0.39
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	6	0.39
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	1	0.39
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	4	0.39
(2,3038)	1:90:A:ALA:H	1:89:A:LYS:HD2	8	0.39
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	15	0.39
(2,2874)	1:118:A:LEU:HD21	1:48:A:GLU:HG3	4	0.39
(2,2874)	1:118:A:LEU:HD23	1:48:A:GLU:HG3	18	0.39
(2,2841)	1:106:A:VAL:HG12	1:105:A:ASN:HB3	8	0.39
(2,2651)	1:22:A:VAL:HG12	1:31:A:LYS:HE3	12	0.39
(2,2542)	1:115:A:TYR:HD2	1:111:A:LEU:HB2	4	0.39
(2,2542)	1:115:A:TYR:HD2	1:111:A:LEU:HB2	7	0.39
(2,2496)	1:46:A:LYS:HG3	1:30:A:GLY:HA2	1	0.39
(2,2376)	1:34:A:ILE:HD13	1:42:A:HIS:HA	10	0.39
(2,2364)	1:93:A:ILE:HG23	1:90:A:ALA:HA	20	0.39
(2,2338)	1:72:A:LYS:HD3	1:79:A:TYR:HA	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2318)	1:50:A:GLU:HB2	1:47:A:ASP:HA	17	0.39
(2,2174)	1:99:A:ILE:HD13	1:89:A:LYS:HA	7	0.39
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	5	0.39
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	7	0.39
(2,1904)	1:56:A:ILE:HD11	1:53:A:SER:HA	6	0.39
(2,1904)	1:56:A:ILE:HD12	1:53:A:SER:HA	9	0.39
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	5	0.39
(2,1847)	1:78:A:GLU:HB3	1:73:A:SER:HB2	8	0.39
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	2	0.39
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	5	0.39
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	7	0.39
(2,1808)	1:92:A:SER:HB3	1:91:A:ILE:HA	8	0.39
(2,1686)	1:24:A:ILE:HG23	1:23:A:THR:HB	13	0.39
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	7	0.39
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	7	0.39
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	13	0.39
(2,1255)	1:28:A:LEU:HD22	1:54:A:SER:H	13	0.39
(2,1255)	1:52:A:LEU:HD13	1:54:A:SER:H	18	0.39
(2,1248)	1:94:A:LEU:HD13	1:95:A:LEU:H	4	0.39
(2,1240)	1:112:A:LEU:HD13	1:113:A:ARG:H	7	0.39
(2,1236)	1:36:A:LEU:HD11	1:38:A:ASN:H	9	0.39
(2,1228)	1:123:A:LEU:HD21	1:124:A:SER:H	1	0.39
(2,1225)	1:95:A:LEU:HD21	1:95:A:LEU:H	6	0.39
(2,1056)	1:91:A:ILE:HG21	1:92:A:SER:H	18	0.39
(2,1056)	1:91:A:ILE:HG21	1:92:A:SER:H	20	0.39
(2,1036)	1:43:A:GLU:HG2	1:33:A:LYS:H	3	0.39
(2,1027)	1:90:A:ALA:HB1	1:92:A:SER:H	14	0.39
(2,1017)	1:45:A:LYS:HD3	1:117:A:SER:H	14	0.39
(2,1017)	1:45:A:LYS:HD3	1:117:A:SER:H	19	0.39
(2,962)	1:95:A:LEU:HA	1:97:A:ARG:H	17	0.39
(2,882)	1:28:A:LEU:HD23	1:28:A:LEU:H	13	0.39
(2,874)	1:49:A:VAL:HG23	1:48:A:GLU:H	18	0.39
(2,868)	1:23:A:THR:HG21	1:24:A:ILE:H	2	0.39
(2,864)	1:111:A:LEU:HD13	1:111:A:LEU:H	9	0.39
(2,851)	1:106:A:VAL:HG13	1:108:A:VAL:H	11	0.39
(2,848)	1:27:A:ALA:HB1	1:26:A:ASP:H	14	0.39
(2,831)	1:112:A:LEU:HD13	1:112:A:LEU:H	8	0.39
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	11	0.39
(2,598)	1:24:A:ILE:HG22	1:52:A:LEU:H	12	0.39
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	12	0.39
(2,580)	1:46:A:LYS:HG3	1:51:A:LYS:H	19	0.39
(2,396)	1:120:A:PHE:HE1	1:68:A:PHE:H	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:22:A:VAL:HG11	1:31:A:LYS:H	14	0.39
(2,166)	1:22:A:VAL:HG12	1:31:A:LYS:H	14	0.39
(2,166)	1:22:A:VAL:HG13	1:31:A:LYS:H	14	0.39
(2,80)	1:34:A:ILE:HG22	1:35:A:ARG:H	4	0.39
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE2	12	0.38
(2,4667)	1:94:A:LEU:HD21	1:115:A:TYR:HE1	5	0.38
(2,4667)	1:94:A:LEU:HD23	1:115:A:TYR:HE2	6	0.38
(2,4570)	1:60:A:LEU:HD21	1:86:A:TRP:HD1	13	0.38
(2,4519)	1:119:A:ILE:HG21	1:68:A:PHE:HD2	2	0.38
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	12	0.38
(2,4465)	1:118:A:LEU:HD11	1:115:A:TYR:HD2	1	0.38
(2,4459)	1:33:A:LYS:HB3	1:41:A:TYR:HD1	13	0.38
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	2	0.38
(2,4457)	1:20:A:GLU:HG3	1:21:A:TYR:HD2	12	0.38
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	18	0.38
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD11	1	0.38
(2,4327)	1:25:A:LYS:H	1:24:A:ILE:HD11	12	0.38
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB1	15	0.38
(2,4315)	1:56:A:ILE:HB	1:90:A:ALA:HB2	20	0.38
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	16	0.38
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD12	8	0.38
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD12	14	0.38
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD12	17	0.38
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD13	6	0.38
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD11	12	0.38
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD11	20	0.38
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD12	20	0.38
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG23	10	0.38
(2,4046)	1:24:A:ILE:HD12	1:66:A:ILE:HG22	16	0.38
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG22	5	0.38
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG22	17	0.38
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG22	14	0.38
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG22	6	0.38
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG23	13	0.38
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG21	19	0.38
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG21	9	0.38
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG23	19	0.38
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG11	16	0.38
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	13	0.38
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	13	0.38
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	13	0.38
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD21	14	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG23	2	0.38
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG22	12	0.38
(2,3601)	1:118:A:LEU:HB3	1:52:A:LEU:HD22	6	0.38
(2,3471)	1:118:A:LEU:HA	1:44:A:ILE:HG12	5	0.38
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	12	0.38
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	6	0.38
(2,3247)	1:60:A:LEU:HD23	1:89:A:LYS:HB3	20	0.38
(2,3050)	1:143:A:HIS:HD2	1:143:A:HIS:HB3	16	0.38
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	7	0.38
(2,2874)	1:118:A:LEU:HD22	1:48:A:GLU:HG3	16	0.38
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	1	0.38
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	6	0.38
(2,2542)	1:115:A:TYR:HD1	1:111:A:LEU:HB2	14	0.38
(2,2382)	1:103:A:ILE:HG23	1:107:A:ASP:HA	3	0.38
(2,2382)	1:103:A:ILE:HG21	1:107:A:ASP:HA	13	0.38
(2,2194)	1:28:A:LEU:HD12	1:54:A:SER:HA	7	0.38
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	5	0.38
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	15	0.38
(2,1904)	1:56:A:ILE:HD13	1:53:A:SER:HA	5	0.38
(2,1891)	1:63:A:LEU:HD23	1:62:A:SER:HB3	18	0.38
(2,1877)	1:137:A:GLU:HB2	1:136:A:SER:HB2	5	0.38
(2,1874)	1:69:A:ILE:HG13	1:82:A:SER:HB3	8	0.38
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	1	0.38
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	3	0.38
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	13	0.38
(2,1686)	1:24:A:ILE:HG22	1:23:A:THR:HB	8	0.38
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	19	0.38
(2,1626)	1:139:A:LEU:HD13	1:136:A:SER:H	4	0.38
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	9	0.38
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	18	0.38
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	3	0.38
(2,1256)	1:24:A:ILE:HG22	1:54:A:SER:H	6	0.38
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	19	0.38
(2,1236)	1:36:A:LEU:HD13	1:38:A:ASN:H	17	0.38
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	7	0.38
(2,1056)	1:91:A:ILE:HG22	1:92:A:SER:H	5	0.38
(2,1036)	1:43:A:GLU:HG2	1:33:A:LYS:H	13	0.38
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	14	0.38
(2,877)	1:60:A:LEU:HD23	1:86:A:TRP:H	10	0.38
(2,874)	1:49:A:VAL:HG21	1:48:A:GLU:H	5	0.38
(2,864)	1:111:A:LEU:HD12	1:111:A:LEU:H	4	0.38
(2,864)	1:111:A:LEU:HD12	1:111:A:LEU:H	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,864)	1:111:A:LEU:HD11	1:111:A:LEU:H	20	0.38
(2,851)	1:106:A:VAL:HG11	1:108:A:VAL:H	8	0.38
(2,848)	1:27:A:ALA:HB3	1:26:A:ASP:H	5	0.38
(2,848)	1:27:A:ALA:HB3	1:26:A:ASP:H	13	0.38
(2,831)	1:119:A:ILE:HD12	1:112:A:LEU:H	13	0.38
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	7	0.38
(2,583)	1:94:A:LEU:HD22	1:55:A:ARG:H	16	0.38
(2,527)	1:72:A:LYS:HB2	1:79:A:TYR:H	11	0.38
(2,396)	1:68:A:PHE:HZ	1:68:A:PHE:H	8	0.38
(2,348)	1:58:A:LEU:HD23	1:61:A:TRP:H	17	0.38
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	2	0.38
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	2	0.38
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	2	0.38
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	16	0.38
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	16	0.38
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	16	0.38
(2,154)	1:71:A:ILE:HD11	1:122:A:ILE:H	6	0.38
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	13	0.38
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	14	0.38
(2,77)	1:56:A:ILE:HD13	1:61:A:TRP:HE1	14	0.38
(2,34)	1:71:A:ILE:HG23	1:72:A:LYS:H	7	0.38
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE2	17	0.37
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	20	0.37
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD12	16	0.37
(2,4276)	1:111:A:LEU:HD21	1:114:A:GLU:HB2	10	0.37
(2,4236)	1:118:A:LEU:HD21	1:117:A:SER:HA	12	0.37
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	20	0.37
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD13	20	0.37
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD11	19	0.37
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD13	20	0.37
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD11	7	0.37
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	16	0.37
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	16	0.37
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	16	0.37
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD12	1	0.37
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD13	5	0.37
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG23	14	0.37
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD11	19	0.37
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG23	3	0.37
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG23	9	0.37
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG21	17	0.37
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG22	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG21	8	0.37
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG21	20	0.37
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB1	17	0.37
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB3	1	0.37
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG22	15	0.37
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG11	7	0.37
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG21	4	0.37
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG22	18	0.37
(2,3716)	1:61:A:TRP:HE3	1:28:A:LEU:HD23	11	0.37
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG13	16	0.37
(2,3625)	1:25:A:LYS:HB2	1:28:A:LEU:HD12	9	0.37
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD23	14	0.37
(2,3389)	1:41:A:TYR:HD2	1:36:A:LEU:HG	16	0.37
(2,3371)	1:48:A:GLU:H	1:118:A:LEU:HD23	12	0.37
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	5	0.37
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	7	0.37
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	12	0.37
(2,3247)	1:60:A:LEU:HD23	1:89:A:LYS:HB3	3	0.37
(2,3201)	1:115:A:TYR:HB2	1:114:A:GLU:HB2	19	0.37
(2,3111)	1:22:A:VAL:HA	1:65:A:LYS:HD3	1	0.37
(2,3111)	1:79:A:TYR:HA	1:72:A:LYS:HD3	9	0.37
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	17	0.37
(2,2874)	1:118:A:LEU:HD23	1:48:A:GLU:HG3	6	0.37
(2,2841)	1:106:A:VAL:HG11	1:105:A:ASN:HB3	11	0.37
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	16	0.37
(2,2653)	1:95:A:LEU:HD13	1:107:A:ASP:HB2	13	0.37
(2,2560)	1:120:A:PHE:HE1	1:34:A:ILE:HB	7	0.37
(2,2376)	1:34:A:ILE:HD12	1:42:A:HIS:HA	16	0.37
(2,2364)	1:93:A:ILE:HG22	1:90:A:ALA:HA	15	0.37
(2,2338)	1:72:A:LYS:HD3	1:79:A:TYR:HA	9	0.37
(2,2074)	1:25:A:LYS:HE2	1:25:A:LYS:HA	8	0.37
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	7	0.37
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	12	0.37
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	16	0.37
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	18	0.37
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	19	0.37
(2,1904)	1:56:A:ILE:HD13	1:53:A:SER:HA	8	0.37
(2,1904)	1:56:A:ILE:HD12	1:53:A:SER:HA	19	0.37
(2,1861)	1:45:A:LYS:HG2	1:117:A:SER:HB2	14	0.37
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	2	0.37
(2,1829)	1:57:A:PRO:HG2	1:57:A:PRO:HA	4	0.37
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1489)	1:8:A:ILE:HG23	1:9:A:GLY:H	1	0.37
(2,1388)	1:34:A:ILE:HG23	1:21:A:TYR:H	19	0.37
(2,1386)	1:65:A:LYS:HD3	1:21:A:TYR:H	12	0.37
(2,1255)	1:52:A:LEU:HD11	1:54:A:SER:H	17	0.37
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	4	0.37
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	5	0.37
(2,1236)	1:19:A:ALA:HB1	1:38:A:ASN:H	6	0.37
(2,1234)	1:94:A:LEU:HD22	1:56:A:ILE:H	3	0.37
(2,1228)	1:123:A:LEU:HD22	1:124:A:SER:H	12	0.37
(2,1225)	1:95:A:LEU:HD22	1:95:A:LEU:H	20	0.37
(2,1219)	1:65:A:LYS:HD2	1:22:A:VAL:H	17	0.37
(2,1082)	1:24:A:ILE:HG23	1:25:A:LYS:H	3	0.37
(2,1056)	1:91:A:ILE:HG22	1:92:A:SER:H	2	0.37
(2,1027)	1:90:A:ALA:HB1	1:92:A:SER:H	8	0.37
(2,895)	1:91:A:ILE:HD11	1:88:A:LYS:H	10	0.37
(2,895)	1:91:A:ILE:HD12	1:88:A:LYS:H	11	0.37
(2,895)	1:91:A:ILE:HD12	1:88:A:LYS:H	14	0.37
(2,882)	1:28:A:LEU:HD21	1:28:A:LEU:H	2	0.37
(2,877)	1:60:A:LEU:HD23	1:86:A:TRP:H	3	0.37
(2,874)	1:49:A:VAL:HG23	1:48:A:GLU:H	12	0.37
(2,864)	1:111:A:LEU:HD13	1:111:A:LEU:H	3	0.37
(2,864)	1:111:A:LEU:HD12	1:111:A:LEU:H	16	0.37
(2,864)	1:111:A:LEU:HD12	1:111:A:LEU:H	17	0.37
(2,851)	1:106:A:VAL:HG11	1:108:A:VAL:H	18	0.37
(2,850)	1:139:A:LEU:HD11	1:140:A:GLU:H	13	0.37
(2,841)	1:139:A:LEU:HD23	1:139:A:LEU:H	3	0.37
(2,663)	1:115:A:TYR:HD2	1:112:A:LEU:H	6	0.37
(2,605)	1:28:A:LEU:HD23	1:51:A:LYS:H	11	0.37
(2,583)	1:94:A:LEU:HD22	1:55:A:ARG:H	10	0.37
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	11	0.37
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	13	0.37
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	6	0.37
(2,560)	1:95:A:LEU:HD11	1:104:A:LEU:H	9	0.37
(2,160)	1:121:A:ILE:HG22	1:70:A:PHE:H	7	0.37
(2,160)	1:121:A:ILE:HG22	1:70:A:PHE:H	15	0.37
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	10	0.37
(2,4667)	1:111:A:LEU:HD21	1:115:A:TYR:HE1	14	0.36
(2,4519)	1:119:A:ILE:HG22	1:68:A:PHE:HD2	6	0.36
(2,4519)	1:119:A:ILE:HG21	1:68:A:PHE:HD1	11	0.36
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE2	16	0.36
(2,4459)	1:33:A:LYS:HB3	1:41:A:TYR:HD2	4	0.36
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD2	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD12	18	0.36
(2,4254)	1:45:A:LYS:HG3	1:47:A:ASP:HB3	7	0.36
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	17	0.36
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD12	9	0.36
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD13	6	0.36
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD12	7	0.36
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD11	12	0.36
(2,4093)	1:120:A:PHE:HD2	1:122:A:ILE:HD12	5	0.36
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD11	17	0.36
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD13	18	0.36
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD13	19	0.36
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD12	15	0.36
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG23	2	0.36
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG22	13	0.36
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG23	20	0.36
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG22	3	0.36
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG22	17	0.36
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB1	4	0.36
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB3	13	0.36
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG23	10	0.36
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG21	19	0.36
(2,3836)	1:90:A:ALA:HB2	1:64:A:VAL:HG12	3	0.36
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	8	0.36
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	8	0.36
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	8	0.36
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	10	0.36
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	10	0.36
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	10	0.36
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD23	5	0.36
(2,3670)	1:103:A:ILE:H	1:104:A:LEU:HD22	6	0.36
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD23	1	0.36
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD23	3	0.36
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD22	10	0.36
(2,3435)	1:22:A:VAL:HA	1:65:A:LYS:HG3	17	0.36
(2,3050)	1:142:A:HIS:HD2	1:142:A:HIS:HB3	6	0.36
(2,2874)	1:118:A:LEU:HD22	1:48:A:GLU:HG3	1	0.36
(2,2863)	1:22:A:VAL:HG12	1:26:A:ASP:HB3	8	0.36
(2,2819)	1:81:A:VAL:HB	1:101:A:ASN:HB2	1	0.36
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	3	0.36
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	4	0.36
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	17	0.36
(2,2653)	1:95:A:LEU:HD11	1:107:A:ASP:HB2	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2538)	1:115:A:TYR:HD1	1:118:A:LEU:HB3	11	0.36
(2,2490)	1:31:A:LYS:HG3	1:30:A:GLY:HA3	1	0.36
(2,2490)	1:31:A:LYS:HG2	1:30:A:GLY:HA3	15	0.36
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	10	0.36
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	17	0.36
(2,2376)	1:34:A:ILE:HD11	1:42:A:HIS:HA	7	0.36
(2,2376)	1:34:A:ILE:HD13	1:42:A:HIS:HA	8	0.36
(2,2175)	1:94:A:LEU:HD22	1:52:A:LEU:HA	18	0.36
(2,2143)	1:133:A:THR:HG22	1:134:A:GLU:HA	11	0.36
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	18	0.36
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	19	0.36
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	4	0.36
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	13	0.36
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	17	0.36
(2,1877)	1:137:A:GLU:HB2	1:136:A:SER:HB2	4	0.36
(2,1877)	1:135:A:LEU:HB3	1:136:A:SER:HB3	10	0.36
(2,1818)	1:88:A:LYS:HE2	1:81:A:VAL:HA	1	0.36
(2,1818)	1:80:A:PHE:HB2	1:81:A:VAL:HA	13	0.36
(2,1781)	1:68:A:PHE:HE1	1:91:A:ILE:HA	3	0.36
(2,1781)	1:68:A:PHE:HE2	1:91:A:ILE:HA	20	0.36
(2,1686)	1:24:A:ILE:HG22	1:23:A:THR:HB	20	0.36
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	13	0.36
(2,1626)	1:135:A:LEU:HD13	1:136:A:SER:H	14	0.36
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	4	0.36
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	11	0.36
(2,1499)	1:93:A:ILE:HG23	1:96:A:GLY:H	1	0.36
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	20	0.36
(2,1236)	1:36:A:LEU:HD11	1:38:A:ASN:H	4	0.36
(2,1228)	1:122:A:ILE:HG23	1:124:A:SER:H	11	0.36
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	8	0.36
(2,1180)	1:45:A:LYS:HE3	1:47:A:ASP:H	1	0.36
(2,1180)	1:45:A:LYS:HE2	1:47:A:ASP:H	6	0.36
(2,1180)	1:26:A:ASP:HB3	1:22:A:VAL:H	8	0.36
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	12	0.36
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	18	0.36
(2,1056)	1:91:A:ILE:HG22	1:92:A:SER:H	1	0.36
(2,1056)	1:91:A:ILE:HG21	1:92:A:SER:H	6	0.36
(2,1056)	1:91:A:ILE:HG21	1:92:A:SER:H	13	0.36
(2,895)	1:91:A:ILE:HD12	1:88:A:LYS:H	20	0.36
(2,885)	1:66:A:ILE:HD13	1:26:A:ASP:H	10	0.36
(2,851)	1:106:A:VAL:HG13	1:108:A:VAL:H	1	0.36
(2,851)	1:106:A:VAL:HG11	1:108:A:VAL:H	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,851)	1:106:A:VAL:HG11	1:108:A:VAL:H	16	0.36
(2,850)	1:139:A:LEU:HD23	1:140:A:GLU:H	6	0.36
(2,841)	1:139:A:LEU:HD22	1:139:A:LEU:H	11	0.36
(2,841)	1:5:A:ILE:HD13	1:5:A:ILE:H	16	0.36
(2,665)	1:115:A:TYR:HE1	1:112:A:LEU:H	20	0.36
(2,607)	1:66:A:ILE:HG23	1:64:A:VAL:H	10	0.36
(2,564)	1:104:A:LEU:HD23	1:79:A:TYR:H	5	0.36
(2,560)	1:95:A:LEU:HD13	1:104:A:LEU:H	10	0.36
(2,516)	1:72:A:LYS:HD2	1:80:A:PHE:H	4	0.36
(2,516)	1:72:A:LYS:HD2	1:80:A:PHE:H	18	0.36
(2,396)	1:120:A:PHE:HE2	1:68:A:PHE:H	6	0.36
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	17	0.36
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	17	0.36
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	17	0.36
(2,154)	1:71:A:ILE:HD13	1:122:A:ILE:H	9	0.36
(2,116)	1:82:A:SER:HB2	1:120:A:PHE:H	20	0.36
(2,83)	1:34:A:ILE:HD13	1:43:A:GLU:H	3	0.36
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	3	0.36
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	6	0.36
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	11	0.36
(2,34)	1:71:A:ILE:HG21	1:72:A:LYS:H	11	0.36
(2,34)	1:71:A:ILE:HG22	1:72:A:LYS:H	13	0.36
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE2	5	0.35
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE1	19	0.35
(2,4648)	1:20:A:GLU:HA	1:21:A:TYR:HE2	15	0.35
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE2	2	0.35
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	3	0.35
(2,4570)	1:60:A:LEU:HD22	1:86:A:TRP:HD1	2	0.35
(2,4551)	1:122:A:ILE:HD12	1:120:A:PHE:HE2	8	0.35
(2,4519)	1:119:A:ILE:HG22	1:68:A:PHE:HD1	1	0.35
(2,4519)	1:119:A:ILE:HG21	1:68:A:PHE:HD2	18	0.35
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE2	10	0.35
(2,4469)	1:69:A:ILE:HD12	1:21:A:TYR:HD2	11	0.35
(2,4469)	1:69:A:ILE:HD13	1:21:A:TYR:HD2	12	0.35
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD2	6	0.35
(2,4438)	1:35:A:ARG:HD3	1:41:A:TYR:HD1	18	0.35
(2,4398)	1:113:A:ARG:HA	1:113:A:ARG:HD2	17	0.35
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB2	17	0.35
(2,4236)	1:118:A:LEU:HD23	1:117:A:SER:HA	16	0.35
(2,4223)	1:69:A:ILE:HG13	1:82:A:SER:HB2	15	0.35
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD12	14	0.35
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD11	20	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD12	20	0.35
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD13	20	0.35
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD13	4	0.35
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD13	10	0.35
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG21	4	0.35
(2,4011)	1:68:A:PHE:HB3	1:119:A:ILE:HG23	8	0.35
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG23	5	0.35
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG23	18	0.35
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG21	6	0.35
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	14	0.35
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	14	0.35
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	14	0.35
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD22	20	0.35
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG11	13	0.35
(2,3635)	1:52:A:LEU:HD11	1:56:A:ILE:HG12	13	0.35
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD23	7	0.35
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	8	0.35
(2,3347)	1:120:A:PHE:HD1	1:69:A:ILE:HG12	18	0.35
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	14	0.35
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD21	19	0.35
(2,3299)	1:44:A:ILE:H	1:33:A:LYS:HG2	12	0.35
(2,2960)	1:52:A:LEU:HA	1:114:A:GLU:HG3	7	0.35
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	18	0.35
(2,2658)	1:81:A:VAL:HG22	1:79:A:TYR:HB2	11	0.35
(2,2494)	1:10:A:LEU:HB2	1:9:A:GLY:HA2	6	0.35
(2,2490)	1:31:A:LYS:HG2	1:30:A:GLY:HA3	9	0.35
(2,2490)	1:31:A:LYS:HG3	1:30:A:GLY:HA3	16	0.35
(2,2175)	1:94:A:LEU:HD22	1:52:A:LEU:HA	16	0.35
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	10	0.35
(2,1904)	1:56:A:ILE:HD12	1:53:A:SER:HA	10	0.35
(2,1877)	1:135:A:LEU:HB3	1:136:A:SER:HB3	2	0.35
(2,1808)	1:95:A:LEU:HA	1:91:A:ILE:HA	4	0.35
(2,1686)	1:24:A:ILE:HG22	1:23:A:THR:HB	2	0.35
(2,1660)	1:130:A:THR:HG21	1:132:A:GLU:H	3	0.35
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	14	0.35
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	2	0.35
(2,1557)	1:24:A:ILE:HD11	1:61:A:TRP:HE1	5	0.35
(2,1542)	1:28:A:LEU:HB2	1:30:A:GLY:H	5	0.35
(2,1540)	1:31:A:LYS:HB3	1:30:A:GLY:H	4	0.35
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	18	0.35
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	20	0.35
(2,1236)	1:36:A:LEU:HD11	1:38:A:ASN:H	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1236)	1:19:A:ALA:HB1	1:38:A:ASN:H	2	0.35
(2,1236)	1:19:A:ALA:HB2	1:38:A:ASN:H	3	0.35
(2,1228)	1:123:A:LEU:HD21	1:124:A:SER:H	3	0.35
(2,1225)	1:95:A:LEU:HD22	1:95:A:LEU:H	10	0.35
(2,1220)	1:99:A:ILE:HG13	1:101:A:ASN:H	16	0.35
(2,1200)	1:36:A:LEU:HB3	1:41:A:TYR:H	11	0.35
(2,1082)	1:24:A:ILE:HG22	1:25:A:LYS:H	4	0.35
(2,1082)	1:24:A:ILE:HG21	1:25:A:LYS:H	6	0.35
(2,1017)	1:45:A:LYS:HD3	1:117:A:SER:H	15	0.35
(2,895)	1:91:A:ILE:HD12	1:88:A:LYS:H	5	0.35
(2,874)	1:49:A:VAL:HG23	1:48:A:GLU:H	1	0.35
(2,874)	1:49:A:VAL:HG23	1:48:A:GLU:H	20	0.35
(2,864)	1:111:A:LEU:HD11	1:111:A:LEU:H	10	0.35
(2,848)	1:27:A:ALA:HB2	1:26:A:ASP:H	8	0.35
(2,841)	1:139:A:LEU:HD21	1:139:A:LEU:H	2	0.35
(2,841)	1:5:A:ILE:HD11	1:5:A:ILE:H	9	0.35
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	10	0.35
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	20	0.35
(2,576)	1:133:A:THR:HG21	1:137:A:GLU:H	6	0.35
(2,564)	1:104:A:LEU:HD22	1:79:A:TYR:H	20	0.35
(2,560)	1:95:A:LEU:HD13	1:104:A:LEU:H	14	0.35
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	18	0.35
(2,510)	1:65:A:LYS:HE2	1:64:A:VAL:H	9	0.35
(2,396)	1:120:A:PHE:HE1	1:68:A:PHE:H	10	0.35
(2,166)	1:22:A:VAL:HG11	1:31:A:LYS:H	8	0.35
(2,166)	1:22:A:VAL:HG12	1:31:A:LYS:H	8	0.35
(2,166)	1:22:A:VAL:HG13	1:31:A:LYS:H	8	0.35
(2,95)	1:70:A:PHE:HD2	1:122:A:ILE:H	7	0.35
(2,84)	1:24:A:ILE:HG21	1:61:A:TRP:HE1	11	0.35
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	2	0.35
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	12	0.35
(2,4696)	1:140:A:GLU:HB3	1:141:A:HIS:HD2	16	0.34
(2,4648)	1:20:A:GLU:HA	1:21:A:TYR:HE2	5	0.34
(2,4648)	1:20:A:GLU:HA	1:21:A:TYR:HE1	12	0.34
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE2	6	0.34
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	13	0.34
(2,4519)	1:119:A:ILE:HG21	1:68:A:PHE:HD2	12	0.34
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE2	18	0.34
(2,4465)	1:118:A:LEU:HD11	1:115:A:TYR:HD1	11	0.34
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD1	3	0.34
(2,4378)	1:46:A:LYS:HG2	1:50:A:GLU:HG2	9	0.34
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD13	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB1	3	0.34
(2,4223)	1:71:A:ILE:HG13	1:82:A:SER:HB2	18	0.34
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD13	13	0.34
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD11	9	0.34
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD11	13	0.34
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	10	0.34
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	10	0.34
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	10	0.34
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD11	5	0.34
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD13	11	0.34
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD13	19	0.34
(2,4116)	1:115:A:TYR:HA	1:119:A:ILE:HD11	3	0.34
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD13	4	0.34
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD13	6	0.34
(2,4087)	1:14:A:PHE:HD1	1:13:A:ILE:HD11	8	0.34
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD13	2	0.34
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD13	3	0.34
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD11	16	0.34
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD11	11	0.34
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD11	5	0.34
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG23	15	0.34
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG21	15	0.34
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG23	12	0.34
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG21	1	0.34
(2,3889)	1:28:A:LEU:H	1:22:A:VAL:HG22	5	0.34
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG22	15	0.34
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG21	18	0.34
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG11	18	0.34
(2,3836)	1:31:A:LYS:HD2	1:22:A:VAL:HG11	1	0.34
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	15	0.34
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	15	0.34
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	15	0.34
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	16	0.34
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	16	0.34
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	16	0.34
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD22	10	0.34
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG12	9	0.34
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD22	2	0.34
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD22	9	0.34
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG11	1	0.34
(2,3670)	1:103:A:ILE:H	1:104:A:LEU:HD23	4	0.34
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG13	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG13	11	0.34
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG23	7	0.34
(2,3471)	1:118:A:LEU:HA	1:44:A:ILE:HG12	10	0.34
(2,3471)	1:32:A:LEU:HA	1:44:A:ILE:HG13	16	0.34
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD12	19	0.34
(2,3435)	1:22:A:VAL:HA	1:65:A:LYS:HG3	16	0.34
(2,3344)	1:70:A:PHE:HD1	1:119:A:ILE:HG12	14	0.34
(2,3344)	1:70:A:PHE:HD1	1:119:A:ILE:HG12	17	0.34
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD13	10	0.34
(2,3299)	1:44:A:ILE:H	1:33:A:LYS:HG2	15	0.34
(2,3201)	1:51:A:LYS:HE3	1:114:A:GLU:HB2	6	0.34
(2,3201)	1:115:A:TYR:HB2	1:114:A:GLU:HB2	9	0.34
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	2	0.34
(2,3038)	1:89:A:LYS:H	1:89:A:LYS:HD2	12	0.34
(2,3017)	1:66:A:ILE:H	1:65:A:LYS:HD3	2	0.34
(2,2874)	1:118:A:LEU:HD22	1:48:A:GLU:HG3	14	0.34
(2,2865)	1:104:A:LEU:HD23	1:105:A:ASN:HB3	9	0.34
(2,2827)	1:50:A:GLU:HB2	1:47:A:ASP:HB3	15	0.34
(2,2825)	1:31:A:LYS:HB3	1:26:A:ASP:HB2	4	0.34
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	5	0.34
(2,2653)	1:95:A:LEU:HD11	1:107:A:ASP:HB2	5	0.34
(2,2490)	1:31:A:LYS:HG2	1:30:A:GLY:HA3	5	0.34
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	2	0.34
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	8	0.34
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	9	0.34
(2,2376)	1:34:A:ILE:HD13	1:42:A:HIS:HA	18	0.34
(2,2364)	1:93:A:ILE:HG23	1:90:A:ALA:HA	6	0.34
(2,2364)	1:93:A:ILE:HG22	1:90:A:ALA:HA	12	0.34
(2,2364)	1:93:A:ILE:HG21	1:90:A:ALA:HA	16	0.34
(2,2175)	1:94:A:LEU:HD23	1:52:A:LEU:HA	20	0.34
(2,2143)	1:133:A:THR:HG21	1:134:A:GLU:HA	3	0.34
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	11	0.34
(2,1998)	1:115:A:TYR:HD1	1:112:A:LEU:HA	1	0.34
(2,1899)	1:76:A:ILE:HD12	1:73:A:SER:HB3	3	0.34
(2,1877)	1:137:A:GLU:HB2	1:136:A:SER:HB2	17	0.34
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	17	0.34
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	18	0.34
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	5	0.34
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	1	0.34
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	5	0.34
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	6	0.34
(2,1645)	1:25:A:LYS:HB2	1:63:A:LEU:H	11	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	6	0.34
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	16	0.34
(2,1509)	1:63:A:LEU:HA	1:62:A:SER:H	1	0.34
(2,1509)	1:63:A:LEU:HA	1:62:A:SER:H	8	0.34
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	6	0.34
(2,1435)	1:25:A:LYS:HB3	1:23:A:THR:H	20	0.34
(2,1402)	1:99:A:ILE:HG21	1:101:A:ASN:HD22	16	0.34
(2,1255)	1:28:A:LEU:HD22	1:54:A:SER:H	10	0.34
(2,1253)	1:52:A:LEU:HD11	1:56:A:ILE:H	19	0.34
(2,1248)	1:94:A:LEU:HD13	1:95:A:LEU:H	17	0.34
(2,1240)	1:112:A:LEU:HD13	1:113:A:ARG:H	3	0.34
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	13	0.34
(2,1236)	1:36:A:LEU:HD13	1:38:A:ASN:H	15	0.34
(2,1225)	1:95:A:LEU:HD22	1:95:A:LEU:H	4	0.34
(2,1225)	1:95:A:LEU:HD22	1:95:A:LEU:H	8	0.34
(2,1225)	1:95:A:LEU:HD22	1:95:A:LEU:H	16	0.34
(2,1180)	1:45:A:LYS:HE2	1:47:A:ASP:H	20	0.34
(2,1066)	1:99:A:ILE:HD13	1:97:A:ARG:H	4	0.34
(2,1027)	1:90:A:ALA:HB2	1:92:A:SER:H	13	0.34
(2,974)	1:87:A:ASN:HB3	1:84:A:GLU:H	13	0.34
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	10	0.34
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	4	0.34
(2,877)	1:63:A:LEU:HB2	1:86:A:TRP:H	4	0.34
(2,874)	1:49:A:VAL:HG21	1:48:A:GLU:H	10	0.34
(2,851)	1:106:A:VAL:HG12	1:108:A:VAL:H	14	0.34
(2,841)	1:139:A:LEU:HD22	1:139:A:LEU:H	5	0.34
(2,831)	1:119:A:ILE:HD13	1:112:A:LEU:H	14	0.34
(2,831)	1:119:A:ILE:HD12	1:112:A:LEU:H	17	0.34
(2,816)	1:51:A:LYS:HG2	1:49:A:VAL:H	17	0.34
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	2	0.34
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	3	0.34
(2,663)	1:115:A:TYR:HD1	1:112:A:LEU:H	5	0.34
(2,663)	1:115:A:TYR:HD1	1:112:A:LEU:H	14	0.34
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	11	0.34
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	11	0.34
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	11	0.34
(2,145)	1:122:A:ILE:HG13	1:70:A:PHE:H	3	0.34
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	18	0.34
(2,83)	1:34:A:ILE:HD11	1:43:A:GLU:H	14	0.34
(2,80)	1:34:A:ILE:HG23	1:35:A:ARG:H	7	0.34
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	16	0.34
(2,34)	1:71:A:ILE:HG22	1:72:A:LYS:H	16	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	7	0.34
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE1	7	0.33
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE2	7	0.33
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE2	11	0.33
(2,4648)	1:20:A:GLU:HA	1:21:A:TYR:HE2	7	0.33
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE1	1	0.33
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	5	0.33
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE2	12	0.33
(2,4570)	1:60:A:LEU:HD22	1:86:A:TRP:HD1	7	0.33
(2,4570)	1:60:A:LEU:HD22	1:86:A:TRP:HD1	11	0.33
(2,4469)	1:35:A:ARG:HG3	1:41:A:TYR:HD2	8	0.33
(2,4468)	1:65:A:LYS:HD2	1:21:A:TYR:HD2	16	0.33
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD1	15	0.33
(2,4377)	1:112:A:LEU:HD13	1:109:A:GLU:HG3	3	0.33
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG22	3	0.33
(2,4300)	1:65:A:LYS:HE3	1:63:A:LEU:HD22	13	0.33
(2,4236)	1:118:A:LEU:HD23	1:117:A:SER:HA	5	0.33
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB3	3	0.33
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD11	3	0.33
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD11	14	0.33
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD12	14	0.33
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD13	14	0.33
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD12	11	0.33
(2,4046)	1:24:A:ILE:HD13	1:66:A:ILE:HG23	14	0.33
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG22	1	0.33
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG22	6	0.33
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG22	7	0.33
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG21	5	0.33
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG22	13	0.33
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG23	19	0.33
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG23	18	0.33
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG21	5	0.33
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB3	2	0.33
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB3	12	0.33
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG11	9	0.33
(2,3836)	1:90:A:ALA:HB1	1:64:A:VAL:HG13	4	0.33
(2,3836)	1:90:A:ALA:HB2	1:64:A:VAL:HG11	8	0.33
(2,3826)	1:79:A:TYR:HB2	1:108:A:VAL:HG12	13	0.33
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG23	16	0.33
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG21	19	0.33
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD22	20	0.33
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD23	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG11	2	0.33
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG13	20	0.33
(2,3471)	1:32:A:LEU:HA	1:44:A:ILE:HG13	19	0.33
(2,3435)	1:22:A:VAL:HA	1:65:A:LYS:HG3	20	0.33
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	9	0.33
(2,3085)	1:21:A:TYR:HD1	1:20:A:GLU:HB2	14	0.33
(2,3017)	1:66:A:ILE:H	1:65:A:LYS:HD3	9	0.33
(2,2865)	1:104:A:LEU:HD21	1:105:A:ASN:HB3	8	0.33
(2,2865)	1:104:A:LEU:HD22	1:105:A:ASN:HB3	19	0.33
(2,2842)	1:25:A:LYS:HB2	1:26:A:ASP:HB2	14	0.33
(2,2658)	1:81:A:VAL:HG23	1:79:A:TYR:HB2	8	0.33
(2,2496)	1:46:A:LYS:HG3	1:30:A:GLY:HA2	16	0.33
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	3	0.33
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	18	0.33
(2,2376)	1:34:A:ILE:HD12	1:42:A:HIS:HA	6	0.33
(2,2376)	1:34:A:ILE:HD13	1:42:A:HIS:HA	9	0.33
(2,2376)	1:34:A:ILE:HD12	1:42:A:HIS:HA	11	0.33
(2,2375)	1:104:A:LEU:HD22	1:78:A:GLU:HA	1	0.33
(2,2174)	1:99:A:ILE:HD13	1:89:A:LYS:HA	6	0.33
(2,2081)	1:43:A:GLU:HG3	1:41:A:TYR:HA	10	0.33
(2,2074)	1:61:A:TRP:HB2	1:25:A:LYS:HA	20	0.33
(2,1847)	1:78:A:GLU:HB3	1:73:A:SER:HB2	10	0.33
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	11	0.33
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	17	0.33
(2,1626)	1:135:A:LEU:HD11	1:136:A:SER:H	3	0.33
(2,1626)	1:135:A:LEU:HD22	1:136:A:SER:H	20	0.33
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	3	0.33
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	4	0.33
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	17	0.33
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	18	0.33
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	11	0.33
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	9	0.33
(2,1542)	1:28:A:LEU:HB2	1:30:A:GLY:H	4	0.33
(2,1520)	1:25:A:LYS:HD2	1:62:A:SER:H	9	0.33
(2,1509)	1:63:A:LEU:HA	1:62:A:SER:H	13	0.33
(2,1440)	1:20:A:GLU:HG2	1:35:A:ARG:HE	2	0.33
(2,1435)	1:31:A:LYS:HB3	1:23:A:THR:H	8	0.33
(2,1398)	1:119:A:ILE:HD12	1:114:A:GLU:H	13	0.33
(2,1386)	1:65:A:LYS:HD3	1:21:A:TYR:H	19	0.33
(2,1256)	1:24:A:ILE:HG23	1:54:A:SER:H	7	0.33
(2,1248)	1:94:A:LEU:HD11	1:95:A:LEU:H	5	0.33
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1225)	1:95:A:LEU:HD21	1:95:A:LEU:H	9	0.33
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	15	0.33
(2,1200)	1:36:A:LEU:HB3	1:41:A:TYR:H	8	0.33
(2,1180)	1:45:A:LYS:HE2	1:47:A:ASP:H	12	0.33
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	8	0.33
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	19	0.33
(2,1066)	1:99:A:ILE:HD12	1:97:A:ARG:H	2	0.33
(2,1036)	1:43:A:GLU:HG2	1:33:A:LYS:H	12	0.33
(2,1027)	1:90:A:ALA:HB2	1:92:A:SER:H	2	0.33
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	11	0.33
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	13	0.33
(2,882)	1:28:A:LEU:HD23	1:28:A:LEU:H	7	0.33
(2,864)	1:111:A:LEU:HD11	1:111:A:LEU:H	13	0.33
(2,851)	1:106:A:VAL:HG13	1:108:A:VAL:H	9	0.33
(2,850)	1:139:A:LEU:HD11	1:140:A:GLU:H	2	0.33
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	19	0.33
(2,663)	1:115:A:TYR:HD1	1:112:A:LEU:H	16	0.33
(2,605)	1:28:A:LEU:HD22	1:51:A:LYS:H	9	0.33
(2,583)	1:94:A:LEU:HD21	1:55:A:ARG:H	6	0.33
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	9	0.33
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	13	0.33
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	5	0.33
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	8	0.33
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	14	0.33
(2,348)	1:58:A:LEU:HD23	1:61:A:TRP:H	9	0.33
(2,348)	1:58:A:LEU:HD23	1:61:A:TRP:H	10	0.33
(2,160)	1:121:A:ILE:HG21	1:70:A:PHE:H	2	0.33
(2,156)	1:69:A:ILE:HD12	1:120:A:PHE:H	14	0.33
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	20	0.33
(2,80)	1:34:A:ILE:HG22	1:35:A:ARG:H	6	0.33
(2,67)	1:33:A:LYS:HE2	1:43:A:GLU:H	7	0.33
(2,33)	1:46:A:LYS:HD3	1:46:A:LYS:H	5	0.33
(2,29)	1:48:A:GLU:HG3	1:46:A:LYS:H	16	0.33
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	5	0.33
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE1	15	0.32
(2,4648)	1:20:A:GLU:HA	1:21:A:TYR:HE1	14	0.32
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE1	7	0.32
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE2	14	0.32
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	15	0.32
(2,4519)	1:119:A:ILE:HG21	1:68:A:PHE:HD2	3	0.32
(2,4519)	1:119:A:ILE:HG23	1:68:A:PHE:HD2	4	0.32
(2,4474)	1:36:A:LEU:HD21	1:41:A:TYR:HD2	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4458)	1:34:A:ILE:HB	1:21:A:TYR:HD1	1	0.32
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	3	0.32
(2,4398)	1:52:A:LEU:HA	1:55:A:ARG:HD3	19	0.32
(2,4373)	1:130:A:THR:HG21	1:131:A:GLU:HB3	9	0.32
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD12	1	0.32
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD12	12	0.32
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD12	19	0.32
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD13	12	0.32
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB2	12	0.32
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG21	7	0.32
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG22	12	0.32
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	2	0.32
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	5	0.32
(2,4249)	1:52:A:LEU:HD11	1:55:A:ARG:HD3	1	0.32
(2,4243)	1:102:A:VAL:HG22	1:104:A:LEU:HA	7	0.32
(2,4236)	1:118:A:LEU:HD22	1:117:A:SER:HA	2	0.32
(2,4236)	1:118:A:LEU:HD22	1:117:A:SER:HA	11	0.32
(2,4236)	1:118:A:LEU:HD22	1:117:A:SER:HA	15	0.32
(2,4236)	1:118:A:LEU:HD23	1:117:A:SER:HA	20	0.32
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB3	17	0.32
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD11	12	0.32
(2,4162)	1:80:A:PHE:HB3	1:71:A:ILE:HD12	5	0.32
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD11	6	0.32
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD12	6	0.32
(2,4146)	1:82:A:SER:HB3	1:71:A:ILE:HD13	6	0.32
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG22	4	0.32
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD13	18	0.32
(2,4093)	1:120:A:PHE:HD1	1:122:A:ILE:HD13	13	0.32
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD11	6	0.32
(2,4046)	1:24:A:ILE:HD12	1:66:A:ILE:HG23	20	0.32
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG21	12	0.32
(2,4020)	1:49:A:VAL:HB	1:44:A:ILE:HG23	8	0.32
(2,4020)	1:118:A:LEU:HB3	1:44:A:ILE:HG21	16	0.32
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG21	5	0.32
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG21	8	0.32
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB3	9	0.32
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB2	17	0.32
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG21	19	0.32
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG22	14	0.32
(2,3836)	1:90:A:ALA:HB1	1:64:A:VAL:HG12	5	0.32
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	5	0.32
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	5	0.32
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	9	0.32
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	9	0.32
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	9	0.32
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	11	0.32
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	11	0.32
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	11	0.32
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD21	6	0.32
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG13	9	0.32
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD21	7	0.32
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG22	1	0.32
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG21	16	0.32
(2,3405)	1:115:A:TYR:HE2	1:118:A:LEU:HD13	3	0.32
(2,3344)	1:70:A:PHE:HD2	1:119:A:ILE:HG12	8	0.32
(2,3344)	1:70:A:PHE:HD2	1:119:A:ILE:HG12	18	0.32
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	2	0.32
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD22	1	0.32
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD22	14	0.32
(2,3299)	1:44:A:ILE:H	1:33:A:LYS:HG2	6	0.32
(2,3247)	1:60:A:LEU:HD22	1:89:A:LYS:HB3	16	0.32
(2,3038)	1:90:A:ALA:H	1:89:A:LYS:HD2	11	0.32
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	15	0.32
(2,2658)	1:81:A:VAL:HG22	1:79:A:TYR:HB2	1	0.32
(2,2560)	1:42:A:HIS:HD2	1:34:A:ILE:HB	3	0.32
(2,2496)	1:46:A:LYS:HG3	1:30:A:GLY:HA2	14	0.32
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	7	0.32
(2,2473)	1:69:A:ILE:HD13	1:18:A:PRO:HD3	12	0.32
(2,2376)	1:34:A:ILE:HD12	1:42:A:HIS:HA	1	0.32
(2,2376)	1:34:A:ILE:HD12	1:42:A:HIS:HA	2	0.32
(2,2376)	1:34:A:ILE:HD12	1:42:A:HIS:HA	5	0.32
(2,2376)	1:34:A:ILE:HD12	1:42:A:HIS:HA	20	0.32
(2,2163)	1:102:A:VAL:HG22	1:103:A:ILE:HA	1	0.32
(2,2163)	1:102:A:VAL:HG21	1:103:A:ILE:HA	18	0.32
(2,2144)	1:91:A:ILE:HG13	1:88:A:LYS:HA	13	0.32
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	4	0.32
(2,2099)	1:134:A:GLU:HG2	1:134:A:GLU:HA	8	0.32
(2,2081)	1:43:A:GLU:HG3	1:41:A:TYR:HA	2	0.32
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	10	0.32
(2,1998)	1:115:A:TYR:HD2	1:112:A:LEU:HA	17	0.32
(2,1904)	1:56:A:ILE:HD12	1:53:A:SER:HA	2	0.32
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	6	0.32
(2,1866)	1:139:A:LEU:HB2	1:136:A:SER:HB3	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	3	0.32
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	1	0.32
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	13	0.32
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	20	0.32
(2,1808)	1:92:A:SER:HB3	1:91:A:ILE:HA	6	0.32
(2,1781)	1:68:A:PHE:HE1	1:91:A:ILE:HA	6	0.32
(2,1781)	1:68:A:PHE:HE2	1:91:A:ILE:HA	15	0.32
(2,1781)	1:68:A:PHE:HE2	1:91:A:ILE:HA	17	0.32
(2,1680)	1:125:A:PRO:HB2	1:126:A:THR:HB	16	0.32
(2,1660)	1:130:A:THR:HG21	1:132:A:GLU:H	5	0.32
(2,1626)	1:135:A:LEU:HD12	1:136:A:SER:H	16	0.32
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	5	0.32
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	14	0.32
(2,1509)	1:63:A:LEU:HA	1:62:A:SER:H	5	0.32
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	9	0.32
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	18	0.32
(2,1489)	1:8:A:ILE:HG21	1:9:A:GLY:H	9	0.32
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	6	0.32
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	15	0.32
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	2	0.32
(2,1236)	1:36:A:LEU:HD13	1:38:A:ASN:H	13	0.32
(2,1225)	1:95:A:LEU:HD23	1:95:A:LEU:H	17	0.32
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	1	0.32
(2,1191)	1:131:A:GLU:HG2	1:133:A:THR:H	7	0.32
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	17	0.32
(2,1056)	1:91:A:ILE:HG21	1:92:A:SER:H	9	0.32
(2,1027)	1:90:A:ALA:HB2	1:92:A:SER:H	9	0.32
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	16	0.32
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	16	0.32
(2,895)	1:91:A:ILE:HD11	1:88:A:LYS:H	9	0.32
(2,882)	1:28:A:LEU:HD21	1:28:A:LEU:H	3	0.32
(2,877)	1:60:A:LEU:HD22	1:86:A:TRP:H	17	0.32
(2,831)	1:119:A:ILE:HD11	1:112:A:LEU:H	11	0.32
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	17	0.32
(2,760)	1:41:A:TYR:HB2	1:34:A:ILE:H	14	0.32
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	14	0.32
(2,733)	1:86:A:TRP:HB3	1:90:A:ALA:H	16	0.32
(2,605)	1:28:A:LEU:HD22	1:51:A:LYS:H	13	0.32
(2,598)	1:24:A:ILE:HG21	1:52:A:LEU:H	2	0.32
(2,598)	1:24:A:ILE:HG21	1:52:A:LEU:H	4	0.32
(2,583)	1:94:A:LEU:HD22	1:55:A:ARG:H	8	0.32
(2,583)	1:94:A:LEU:HD23	1:55:A:ARG:H	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	1	0.32
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	3	0.32
(2,571)	1:118:A:LEU:HD12	1:52:A:LEU:H	10	0.32
(2,510)	1:65:A:LYS:HE3	1:64:A:VAL:H	14	0.32
(2,396)	1:120:A:PHE:HE1	1:68:A:PHE:H	20	0.32
(2,348)	1:58:A:LEU:HD21	1:61:A:TRP:H	16	0.32
(2,348)	1:58:A:LEU:HD22	1:61:A:TRP:H	18	0.32
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	19	0.32
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	19	0.32
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	19	0.32
(2,160)	1:121:A:ILE:HG22	1:70:A:PHE:H	20	0.32
(2,145)	1:122:A:ILE:HG13	1:70:A:PHE:H	4	0.32
(2,145)	1:122:A:ILE:HG13	1:70:A:PHE:H	9	0.32
(2,84)	1:24:A:ILE:HG23	1:61:A:TRP:HE1	7	0.32
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	8	0.32
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	2	0.32
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	15	0.32
(2,34)	1:71:A:ILE:HG22	1:72:A:LYS:H	15	0.32
(2,29)	1:48:A:GLU:HG3	1:46:A:LYS:H	13	0.32
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE1	16	0.31
(2,4644)	1:123:A:LEU:HA	1:79:A:TYR:HE2	14	0.31
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE2	4	0.31
(2,4551)	1:69:A:ILE:HD12	1:120:A:PHE:HE1	11	0.31
(2,4551)	1:122:A:ILE:HD12	1:120:A:PHE:HE1	13	0.31
(2,4459)	1:33:A:LYS:HB3	1:41:A:TYR:HD1	1	0.31
(2,4458)	1:20:A:GLU:HB2	1:21:A:TYR:HD1	8	0.31
(2,4414)	1:132:A:GLU:HG2	1:133:A:THR:HB	17	0.31
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	4	0.31
(2,4377)	1:112:A:LEU:HD11	1:109:A:GLU:HG3	16	0.31
(2,4236)	1:118:A:LEU:HD21	1:117:A:SER:HA	17	0.31
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD13	16	0.31
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD13	1	0.31
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD11	19	0.31
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD12	15	0.31
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD12	3	0.31
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD11	17	0.31
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD11	19	0.31
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG23	3	0.31
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD11	20	0.31
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD12	5	0.31
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD11	10	0.31
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4046)	1:24:A:ILE:HD12	1:66:A:ILE:HG21	6	0.31
(2,4046)	1:24:A:ILE:HD13	1:66:A:ILE:HG21	7	0.31
(2,4046)	1:24:A:ILE:HD12	1:66:A:ILE:HG21	17	0.31
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG23	10	0.31
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG21	6	0.31
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG22	9	0.31
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG23	19	0.31
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG22	5	0.31
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG21	10	0.31
(2,3911)	1:70:A:PHE:HE2	1:103:A:ILE:HG23	3	0.31
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG22	4	0.31
(2,3836)	1:90:A:ALA:HB2	1:64:A:VAL:HG11	17	0.31
(2,3799)	1:107:A:ASP:HB3	1:95:A:LEU:HD23	8	0.31
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG13	18	0.31
(2,3635)	1:52:A:LEU:HD13	1:56:A:ILE:HG12	20	0.31
(2,3463)	1:82:A:SER:HA	1:88:A:LYS:HG3	1	0.31
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	20	0.31
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD22	7	0.31
(2,3201)	1:51:A:LYS:HE3	1:114:A:GLU:HB2	2	0.31
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	14	0.31
(2,2915)	1:115:A:TYR:HD1	1:114:A:GLU:HG2	20	0.31
(2,2845)	1:51:A:LYS:HG3	1:47:A:ASP:HB2	9	0.31
(2,2841)	1:106:A:VAL:HG13	1:105:A:ASN:HB2	13	0.31
(2,2819)	1:81:A:VAL:HB	1:101:A:ASN:HB2	11	0.31
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	9	0.31
(2,2658)	1:81:A:VAL:HG23	1:79:A:TYR:HB2	19	0.31
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	2	0.31
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	16	0.31
(2,2175)	1:94:A:LEU:HD21	1:52:A:LEU:HA	8	0.31
(2,2143)	1:133:A:THR:HG21	1:134:A:GLU:HA	17	0.31
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	9	0.31
(2,1904)	1:56:A:ILE:HD13	1:53:A:SER:HA	4	0.31
(2,1904)	1:56:A:ILE:HD11	1:53:A:SER:HA	17	0.31
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	9	0.31
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	7	0.31
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	8	0.31
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	15	0.31
(2,1808)	1:92:A:SER:HB3	1:91:A:ILE:HA	11	0.31
(2,1660)	1:130:A:THR:HG21	1:132:A:GLU:H	12	0.31
(2,1641)	1:58:A:LEU:HB3	1:60:A:LEU:H	19	0.31
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	12	0.31
(2,1541)	1:22:A:VAL:HB	1:30:A:GLY:H	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1499)	1:93:A:ILE:HG22	1:96:A:GLY:H	3	0.31
(2,1350)	1:50:A:GLU:HB3	1:53:A:SER:H	10	0.31
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	3	0.31
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	5	0.31
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	11	0.31
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	1	0.31
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	3	0.31
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	9	0.31
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	16	0.31
(2,1200)	1:36:A:LEU:HB3	1:41:A:TYR:H	13	0.31
(2,1200)	1:36:A:LEU:HB3	1:41:A:TYR:H	18	0.31
(2,1180)	1:45:A:LYS:HE3	1:47:A:ASP:H	3	0.31
(2,1180)	1:26:A:ASP:HB3	1:22:A:VAL:H	10	0.31
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	10	0.31
(2,1056)	1:91:A:ILE:HG21	1:92:A:SER:H	8	0.31
(2,1056)	1:91:A:ILE:HG21	1:92:A:SER:H	16	0.31
(2,962)	1:95:A:LEU:HA	1:97:A:ARG:H	12	0.31
(2,895)	1:91:A:ILE:HD12	1:88:A:LYS:H	19	0.31
(2,885)	1:66:A:ILE:HD11	1:26:A:ASP:H	20	0.31
(2,874)	1:49:A:VAL:HG21	1:48:A:GLU:H	2	0.31
(2,874)	1:49:A:VAL:HG23	1:48:A:GLU:H	13	0.31
(2,874)	1:49:A:VAL:HG23	1:48:A:GLU:H	16	0.31
(2,848)	1:27:A:ALA:HB1	1:26:A:ASP:H	18	0.31
(2,663)	1:115:A:TYR:HD1	1:112:A:LEU:H	8	0.31
(2,663)	1:115:A:TYR:HD2	1:112:A:LEU:H	17	0.31
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	4	0.31
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	9	0.31
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	2	0.31
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	16	0.31
(2,527)	1:72:A:LYS:HB2	1:79:A:TYR:H	13	0.31
(2,517)	1:43:A:GLU:HG3	1:42:A:HIS:H	18	0.31
(2,108)	1:67:A:PRO:HA	1:120:A:PHE:H	20	0.31
(2,83)	1:34:A:ILE:HD11	1:43:A:GLU:H	17	0.31
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE1	12	0.3
(2,4689)	1:123:A:LEU:HD21	1:79:A:TYR:HD2	19	0.3
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE1	15	0.3
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	1	0.3
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE2	11	0.3
(2,4641)	1:78:A:GLU:HA	1:79:A:TYR:HE2	3	0.3
(2,4570)	1:60:A:LEU:HD23	1:86:A:TRP:HD1	5	0.3
(2,4505)	1:122:A:ILE:HG22	1:14:A:PHE:HD1	14	0.3
(2,4459)	1:33:A:LYS:HB3	1:41:A:TYR:HD1	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	18	0.3
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD12	12	0.3
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	18	0.3
(2,4236)	1:118:A:LEU:HD23	1:117:A:SER:HA	7	0.3
(2,4236)	1:118:A:LEU:HD22	1:117:A:SER:HA	10	0.3
(2,4236)	1:118:A:LEU:HD22	1:117:A:SER:HA	19	0.3
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB2	2	0.3
(2,4207)	1:70:A:PHE:HE2	1:91:A:ILE:HD11	3	0.3
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD11	1	0.3
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD13	3	0.3
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD12	15	0.3
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD12	7	0.3
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD12	13	0.3
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD13	2	0.3
(2,4125)	1:102:A:VAL:HA	1:103:A:ILE:HD12	13	0.3
(2,4123)	1:65:A:LYS:HA	1:66:A:ILE:HD13	15	0.3
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD11	9	0.3
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD12	7	0.3
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD13	15	0.3
(2,4011)	1:68:A:PHE:HB3	1:119:A:ILE:HG23	17	0.3
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG22	6	0.3
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG22	16	0.3
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG21	1	0.3
(2,3803)	1:42:A:HIS:HB2	1:36:A:LEU:HD21	4	0.3
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG21	1	0.3
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG23	9	0.3
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	6	0.3
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	6	0.3
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	6	0.3
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG13	15	0.3
(2,3422)	1:71:A:ILE:HA	1:122:A:ILE:HG13	15	0.3
(2,3347)	1:120:A:PHE:HD1	1:69:A:ILE:HG12	10	0.3
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	8	0.3
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD21	9	0.3
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD13	7	0.3
(2,3017)	1:66:A:ILE:H	1:65:A:LYS:HD3	4	0.3
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	16	0.3
(2,2827)	1:45:A:LYS:HB3	1:47:A:ASP:HB3	17	0.3
(2,2653)	1:95:A:LEU:HD11	1:107:A:ASP:HB2	16	0.3
(2,2652)	1:95:A:LEU:HD23	1:107:A:ASP:HB2	11	0.3
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	15	0.3
(2,2538)	1:115:A:TYR:HD1	1:118:A:LEU:HB3	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2496)	1:32:A:LEU:HB2	1:30:A:GLY:HA2	11	0.3
(2,2494)	1:10:A:LEU:HB2	1:9:A:GLY:HA2	14	0.3
(2,2376)	1:34:A:ILE:HD11	1:42:A:HIS:HA	4	0.3
(2,2376)	1:34:A:ILE:HD12	1:42:A:HIS:HA	15	0.3
(2,2375)	1:104:A:LEU:HD21	1:78:A:GLU:HA	16	0.3
(2,2375)	1:104:A:LEU:HD21	1:78:A:GLU:HA	19	0.3
(2,2338)	1:65:A:LYS:HD2	1:21:A:TYR:HA	17	0.3
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	20	0.3
(2,1904)	1:56:A:ILE:HD12	1:53:A:SER:HA	16	0.3
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	1	0.3
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	2	0.3
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	3	0.3
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	9	0.3
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	12	0.3
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	18	0.3
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	19	0.3
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	9	0.3
(2,1632)	1:138:A:MET:HB3	1:136:A:SER:H	17	0.3
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	10	0.3
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	2	0.3
(2,1541)	1:22:A:VAL:HB	1:30:A:GLY:H	8	0.3
(2,1509)	1:63:A:LEU:HA	1:62:A:SER:H	2	0.3
(2,1509)	1:63:A:LEU:HA	1:62:A:SER:H	16	0.3
(2,1388)	1:22:A:VAL:HG13	1:21:A:TYR:H	12	0.3
(2,1388)	1:34:A:ILE:HG22	1:21:A:TYR:H	14	0.3
(2,1350)	1:50:A:GLU:HB3	1:53:A:SER:H	7	0.3
(2,1314)	1:100:A:SER:HB3	1:101:A:ASN:HD21	9	0.3
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	18	0.3
(2,1191)	1:132:A:GLU:HG2	1:133:A:THR:H	9	0.3
(2,1180)	1:26:A:ASP:HB3	1:22:A:VAL:H	14	0.3
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	8	0.3
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	16	0.3
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	10	0.3
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	12	0.3
(2,1082)	1:24:A:ILE:HG22	1:25:A:LYS:H	17	0.3
(2,1063)	1:23:A:THR:HG22	1:25:A:LYS:H	5	0.3
(2,1063)	1:23:A:THR:HG22	1:25:A:LYS:H	9	0.3
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	11	0.3
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	10	0.3
(2,882)	1:28:A:LEU:HD21	1:28:A:LEU:H	11	0.3
(2,877)	1:60:A:LEU:HD21	1:86:A:TRP:H	12	0.3
(2,877)	1:60:A:LEU:HD22	1:86:A:TRP:H	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	6	0.3
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	17	0.3
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	8	0.3
(2,663)	1:115:A:TYR:HD1	1:112:A:LEU:H	12	0.3
(2,583)	1:94:A:LEU:HD22	1:55:A:ARG:H	3	0.3
(2,583)	1:94:A:LEU:HD22	1:55:A:ARG:H	19	0.3
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	6	0.3
(2,560)	1:95:A:LEU:HD11	1:104:A:LEU:H	18	0.3
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	6	0.3
(2,396)	1:120:A:PHE:HE1	1:68:A:PHE:H	2	0.3
(2,396)	1:120:A:PHE:HE2	1:68:A:PHE:H	19	0.3
(2,160)	1:121:A:ILE:HG23	1:70:A:PHE:H	3	0.3
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	11	0.3
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	19	0.3
(2,80)	1:34:A:ILE:HG23	1:35:A:ARG:H	16	0.3
(2,33)	1:46:A:LYS:HD3	1:46:A:LYS:H	1	0.3
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE2	17	0.29
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE1	19	0.29
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE1	6	0.29
(2,4701)	1:128:A:SER:HB2	1:129:A:TYR:HE2	6	0.29
(2,4667)	1:111:A:LEU:HD23	1:115:A:TYR:HE2	7	0.29
(2,4641)	1:78:A:GLU:HA	1:79:A:TYR:HE1	12	0.29
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD1	8	0.29
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD11	2	0.29
(2,4333)	1:18:A:PRO:HD3	1:122:A:ILE:HD12	15	0.29
(2,4333)	1:18:A:PRO:HD3	1:122:A:ILE:HD12	17	0.29
(2,4282)	1:138:A:MET:HA	1:141:A:HIS:HB3	5	0.29
(2,4236)	1:118:A:LEU:HD23	1:117:A:SER:HA	1	0.29
(2,4236)	1:118:A:LEU:HD23	1:117:A:SER:HA	3	0.29
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD13	3	0.29
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD13	8	0.29
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD13	13	0.29
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD12	14	0.29
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD13	18	0.29
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD13	8	0.29
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD11	9	0.29
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD13	13	0.29
(2,4046)	1:24:A:ILE:HD11	1:66:A:ILE:HG23	3	0.29
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG22	8	0.29
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG21	11	0.29
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG22	8	0.29
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG22	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB3	4	0.29
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG22	16	0.29
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG21	6	0.29
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG22	20	0.29
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD22	16	0.29
(2,3635)	1:52:A:LEU:HD12	1:56:A:ILE:HG12	1	0.29
(2,3635)	1:52:A:LEU:HD12	1:56:A:ILE:HG12	4	0.29
(2,3635)	1:52:A:LEU:HD13	1:56:A:ILE:HG12	12	0.29
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG21	20	0.29
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD21	18	0.29
(2,3527)	1:49:A:VAL:HA	1:52:A:LEU:HD21	7	0.29
(2,3471)	1:118:A:LEU:HA	1:44:A:ILE:HG12	3	0.29
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD11	18	0.29
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	14	0.29
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD22	16	0.29
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD13	8	0.29
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD11	14	0.29
(2,3299)	1:44:A:ILE:H	1:33:A:LYS:HG2	18	0.29
(2,3271)	1:28:A:LEU:HD11	1:25:A:LYS:HD3	13	0.29
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	4	0.29
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	8	0.29
(2,2954)	1:137:A:GLU:HA	1:137:A:GLU:HG2	19	0.29
(2,2874)	1:118:A:LEU:HD21	1:48:A:GLU:HG3	13	0.29
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	11	0.29
(2,2658)	1:81:A:VAL:HG22	1:79:A:TYR:HB2	10	0.29
(2,2658)	1:81:A:VAL:HG21	1:79:A:TYR:HB2	13	0.29
(2,2560)	1:42:A:HIS:HD2	1:34:A:ILE:HB	15	0.29
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	8	0.29
(2,2496)	1:32:A:LEU:HB2	1:30:A:GLY:HA2	12	0.29
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	4	0.29
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	12	0.29
(2,2473)	1:122:A:ILE:HD12	1:18:A:PRO:HD3	15	0.29
(2,2473)	1:122:A:ILE:HD12	1:18:A:PRO:HD3	17	0.29
(2,2376)	1:34:A:ILE:HD13	1:42:A:HIS:HA	13	0.29
(2,2194)	1:58:A:LEU:HD21	1:54:A:SER:HA	5	0.29
(2,2141)	1:52:A:LEU:HG	1:52:A:LEU:HA	7	0.29
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	3	0.29
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	2	0.29
(2,2115)	1:36:A:LEU:HB2	1:41:A:TYR:HA	16	0.29
(2,2081)	1:36:A:LEU:HB3	1:41:A:TYR:HA	17	0.29
(2,1904)	1:56:A:ILE:HD11	1:53:A:SER:HA	11	0.29
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	10	0.29
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	14	0.29
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	16	0.29
(2,1808)	1:92:A:SER:HB3	1:91:A:ILE:HA	17	0.29
(2,1781)	1:68:A:PHE:HE2	1:91:A:ILE:HA	11	0.29
(2,1680)	1:125:A:PRO:HB2	1:126:A:THR:HB	10	0.29
(2,1626)	1:135:A:LEU:HD11	1:136:A:SER:H	13	0.29
(2,1541)	1:22:A:VAL:HB	1:30:A:GLY:H	15	0.29
(2,1499)	1:93:A:ILE:HG23	1:96:A:GLY:H	16	0.29
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	15	0.29
(2,1404)	1:69:A:ILE:HD12	1:37:A:ASN:HD22	9	0.29
(2,1401)	1:106:A:VAL:HG21	1:105:A:ASN:HD22	4	0.29
(2,1388)	1:22:A:VAL:HG13	1:21:A:TYR:H	2	0.29
(2,1386)	1:65:A:LYS:HD3	1:21:A:TYR:H	14	0.29
(2,1350)	1:50:A:GLU:HB3	1:53:A:SER:H	16	0.29
(2,1255)	1:28:A:LEU:HD22	1:54:A:SER:H	16	0.29
(2,1248)	1:94:A:LEU:HD13	1:95:A:LEU:H	3	0.29
(2,1248)	1:94:A:LEU:HD12	1:95:A:LEU:H	6	0.29
(2,1248)	1:94:A:LEU:HD12	1:95:A:LEU:H	13	0.29
(2,1240)	1:112:A:LEU:HD13	1:113:A:ARG:H	4	0.29
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	14	0.29
(2,1236)	1:36:A:LEU:HD13	1:38:A:ASN:H	10	0.29
(2,1180)	1:45:A:LYS:HE2	1:47:A:ASP:H	5	0.29
(2,1180)	1:45:A:LYS:HE2	1:47:A:ASP:H	16	0.29
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	15	0.29
(2,1082)	1:24:A:ILE:HG23	1:25:A:LYS:H	14	0.29
(2,1056)	1:91:A:ILE:HG22	1:92:A:SER:H	3	0.29
(2,1056)	1:91:A:ILE:HG22	1:92:A:SER:H	11	0.29
(2,1056)	1:91:A:ILE:HG22	1:92:A:SER:H	14	0.29
(2,1056)	1:91:A:ILE:HG23	1:92:A:SER:H	17	0.29
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	1	0.29
(2,885)	1:66:A:ILE:HD12	1:26:A:ASP:H	15	0.29
(2,882)	1:28:A:LEU:HD23	1:28:A:LEU:H	16	0.29
(2,874)	1:49:A:VAL:HG23	1:48:A:GLU:H	9	0.29
(2,848)	1:27:A:ALA:HB1	1:26:A:ASP:H	16	0.29
(2,841)	1:139:A:LEU:HD21	1:139:A:LEU:H	12	0.29
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	16	0.29
(2,784)	1:61:A:TRP:HB2	1:24:A:ILE:H	8	0.29
(2,764)	1:29:A:ASP:HB3	1:28:A:LEU:H	10	0.29
(2,610)	1:24:A:ILE:HG22	1:63:A:LEU:H	19	0.29
(2,583)	1:94:A:LEU:HD23	1:55:A:ARG:H	17	0.29
(2,564)	1:104:A:LEU:HD13	1:79:A:TYR:H	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,560)	1:95:A:LEU:HD13	1:104:A:LEU:H	20	0.29
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	4	0.29
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	13	0.29
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	19	0.29
(2,527)	1:72:A:LYS:HD3	1:79:A:TYR:H	5	0.29
(2,527)	1:72:A:LYS:HB2	1:79:A:TYR:H	17	0.29
(2,510)	1:65:A:LYS:HE2	1:64:A:VAL:H	2	0.29
(2,348)	1:58:A:LEU:HD22	1:61:A:TRP:H	5	0.29
(2,161)	1:69:A:ILE:HG22	1:70:A:PHE:H	13	0.29
(2,160)	1:121:A:ILE:HG23	1:70:A:PHE:H	8	0.29
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	1	0.29
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	12	0.29
(2,95)	1:70:A:PHE:HD1	1:122:A:ILE:H	20	0.29
(2,84)	1:24:A:ILE:HG21	1:61:A:TRP:HE1	3	0.29
(2,80)	1:34:A:ILE:HG21	1:35:A:ARG:H	3	0.29
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	9	0.29
(2,33)	1:46:A:LYS:HD3	1:46:A:LYS:H	18	0.29
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE1	6	0.28
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE2	13	0.28
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE2	16	0.28
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE2	4	0.28
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE2	4	0.28
(2,4465)	1:118:A:LEU:HD13	1:115:A:TYR:HD1	18	0.28
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	10	0.28
(2,4385)	1:46:A:LYS:HE2	1:50:A:GLU:HG2	4	0.28
(2,4374)	1:135:A:LEU:HD13	1:131:A:GLU:HB2	16	0.28
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD11	9	0.28
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB3	14	0.28
(2,4276)	1:111:A:LEU:HD21	1:114:A:GLU:HB2	17	0.28
(2,4243)	1:102:A:VAL:HG21	1:104:A:LEU:HA	18	0.28
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB2	16	0.28
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD13	2	0.28
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD11	4	0.28
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD11	12	0.28
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD11	16	0.28
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD13	1	0.28
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	2	0.28
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	2	0.28
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	2	0.28
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD13	10	0.28
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD12	15	0.28
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD13	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD11	19	0.28
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD11	12	0.28
(2,4085)	1:24:A:ILE:H	1:24:A:ILE:HD13	15	0.28
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	2	0.28
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG22	12	0.28
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG23	10	0.28
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG22	17	0.28
(2,3973)	1:67:A:PRO:HA	1:119:A:ILE:HG23	4	0.28
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG23	9	0.28
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG21	16	0.28
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG23	2	0.28
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG23	4	0.28
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB1	10	0.28
(2,3836)	1:90:A:ALA:HB3	1:64:A:VAL:HG11	9	0.28
(2,3803)	1:42:A:HIS:HB2	1:36:A:LEU:HD22	5	0.28
(2,3720)	1:86:A:TRP:HH2	1:63:A:LEU:HD22	20	0.28
(2,3714)	1:49:A:VAL:H	1:28:A:LEU:HD21	6	0.28
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG12	1	0.28
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD21	4	0.28
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD21	10	0.28
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG13	4	0.28
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG12	14	0.28
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG22	11	0.28
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD22	11	0.28
(2,3457)	1:76:A:ILE:HA	1:76:A:ILE:HG13	16	0.28
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD12	8	0.28
(2,3422)	1:71:A:ILE:HA	1:122:A:ILE:HG13	17	0.28
(2,3371)	1:48:A:GLU:H	1:118:A:LEU:HD21	8	0.28
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD12	12	0.28
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD21	18	0.28
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	2	0.28
(2,3050)	1:143:A:HIS:HD2	1:143:A:HIS:HB3	2	0.28
(2,3017)	1:66:A:ILE:H	1:65:A:LYS:HD3	18	0.28
(2,2931)	1:41:A:TYR:HD1	1:20:A:GLU:HG2	16	0.28
(2,2915)	1:115:A:TYR:HD2	1:114:A:GLU:HG2	2	0.28
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	15	0.28
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	7	0.28
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	12	0.28
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	14	0.28
(2,2658)	1:81:A:VAL:HG21	1:79:A:TYR:HB2	7	0.28
(2,2653)	1:95:A:LEU:HD13	1:107:A:ASP:HB2	8	0.28
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2542)	1:115:A:TYR:HD2	1:111:A:LEU:HB2	17	0.28
(2,2538)	1:115:A:TYR:HD1	1:118:A:LEU:HB3	2	0.28
(2,2494)	1:10:A:LEU:HG	1:9:A:GLY:HA2	1	0.28
(2,2376)	1:34:A:ILE:HD11	1:42:A:HIS:HA	19	0.28
(2,2163)	1:102:A:VAL:HG22	1:103:A:ILE:HA	9	0.28
(2,2143)	1:133:A:THR:HG23	1:134:A:GLU:HA	15	0.28
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	2	0.28
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	8	0.28
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	20	0.28
(2,2074)	1:61:A:TRP:HB2	1:25:A:LYS:HA	18	0.28
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	8	0.28
(2,1904)	1:56:A:ILE:HD12	1:53:A:SER:HA	13	0.28
(2,1891)	1:63:A:LEU:HD22	1:62:A:SER:HB3	10	0.28
(2,1891)	1:63:A:LEU:HD23	1:62:A:SER:HB3	17	0.28
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	11	0.28
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	7	0.28
(2,1833)	1:51:A:LYS:HB2	1:54:A:SER:HB2	5	0.28
(2,1809)	1:90:A:ALA:HA	1:91:A:ILE:HA	4	0.28
(2,1781)	1:68:A:PHE:HE1	1:91:A:ILE:HA	8	0.28
(2,1660)	1:130:A:THR:HG22	1:132:A:GLU:H	19	0.28
(2,1626)	1:139:A:LEU:HD13	1:136:A:SER:H	15	0.28
(2,1626)	1:135:A:LEU:HD23	1:136:A:SER:H	17	0.28
(2,1621)	1:24:A:ILE:HG12	1:25:A:LYS:H	1	0.28
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	11	0.28
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	12	0.28
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	15	0.28
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	7	0.28
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	11	0.28
(2,1540)	1:31:A:LYS:HB3	1:30:A:GLY:H	6	0.28
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	6	0.28
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	20	0.28
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	17	0.28
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	12	0.28
(2,1447)	1:22:A:VAL:HG22	1:23:A:THR:H	5	0.28
(2,1447)	1:22:A:VAL:HG23	1:23:A:THR:H	13	0.28
(2,1435)	1:31:A:LYS:HB3	1:23:A:THR:H	9	0.28
(2,1435)	1:31:A:LYS:HB3	1:23:A:THR:H	16	0.28
(2,1388)	1:22:A:VAL:HG11	1:21:A:TYR:H	11	0.28
(2,1314)	1:100:A:SER:HB2	1:101:A:ASN:HD21	1	0.28
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	8	0.28
(2,1248)	1:94:A:LEU:HD13	1:95:A:LEU:H	14	0.28
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1225)	1:95:A:LEU:HD21	1:95:A:LEU:H	12	0.28
(2,1180)	1:45:A:LYS:HE3	1:47:A:ASP:H	2	0.28
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	9	0.28
(2,1082)	1:24:A:ILE:HG23	1:25:A:LYS:H	9	0.28
(2,1027)	1:90:A:ALA:HB2	1:92:A:SER:H	18	0.28
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	8	0.28
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	1	0.28
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	19	0.28
(2,885)	1:66:A:ILE:HD11	1:26:A:ASP:H	2	0.28
(2,885)	1:66:A:ILE:HD12	1:26:A:ASP:H	11	0.28
(2,885)	1:66:A:ILE:HD11	1:26:A:ASP:H	12	0.28
(2,882)	1:28:A:LEU:HD23	1:28:A:LEU:H	8	0.28
(2,877)	1:60:A:LEU:HD22	1:86:A:TRP:H	2	0.28
(2,877)	1:60:A:LEU:HD21	1:86:A:TRP:H	14	0.28
(2,877)	1:63:A:LEU:HB2	1:86:A:TRP:H	15	0.28
(2,874)	1:49:A:VAL:HG21	1:48:A:GLU:H	3	0.28
(2,874)	1:49:A:VAL:HG22	1:48:A:GLU:H	6	0.28
(2,850)	1:139:A:LEU:HD12	1:140:A:GLU:H	3	0.28
(2,841)	1:5:A:ILE:HD12	1:5:A:ILE:H	8	0.28
(2,831)	1:119:A:ILE:HD12	1:112:A:LEU:H	1	0.28
(2,819)	1:112:A:LEU:HB2	1:111:A:LEU:H	6	0.28
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	2	0.28
(2,677)	1:78:A:GLU:HA	1:103:A:ILE:H	13	0.28
(2,597)	1:52:A:LEU:HD12	1:52:A:LEU:H	12	0.28
(2,597)	1:52:A:LEU:HD21	1:52:A:LEU:H	18	0.28
(2,583)	1:94:A:LEU:HD22	1:55:A:ARG:H	11	0.28
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	10	0.28
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	19	0.28
(2,571)	1:118:A:LEU:HD12	1:52:A:LEU:H	2	0.28
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	8	0.28
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	1	0.28
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	3	0.28
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	12	0.28
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	17	0.28
(2,160)	1:121:A:ILE:HG23	1:70:A:PHE:H	6	0.28
(2,160)	1:121:A:ILE:HG23	1:70:A:PHE:H	13	0.28
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	17	0.28
(2,80)	1:34:A:ILE:HG23	1:35:A:ARG:H	11	0.28
(2,80)	1:34:A:ILE:HG21	1:35:A:ARG:H	12	0.28
(2,56)	1:57:A:PRO:HD3	1:61:A:TRP:HE1	7	0.28
(2,34)	1:71:A:ILE:HG21	1:72:A:LYS:H	20	0.28
(2,33)	1:45:A:LYS:HD2	1:46:A:LYS:H	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	18	0.28
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE2	10	0.27
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE1	11	0.27
(2,4667)	1:94:A:LEU:HD22	1:115:A:TYR:HE2	4	0.27
(2,4642)	1:21:A:TYR:HA	1:21:A:TYR:HE1	19	0.27
(2,4474)	1:36:A:LEU:HD22	1:41:A:TYR:HD1	15	0.27
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD2	6	0.27
(2,4459)	1:33:A:LYS:HB3	1:41:A:TYR:HD2	8	0.27
(2,4385)	1:46:A:LYS:HE2	1:50:A:GLU:HG2	11	0.27
(2,4351)	1:111:A:LEU:HD23	1:91:A:ILE:HD11	13	0.27
(2,4320)	1:24:A:ILE:HB	1:66:A:ILE:HG22	15	0.27
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG22	13	0.27
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	9	0.27
(2,4236)	1:118:A:LEU:HD22	1:117:A:SER:HA	4	0.27
(2,4236)	1:118:A:LEU:HD22	1:117:A:SER:HA	13	0.27
(2,4236)	1:118:A:LEU:HD21	1:117:A:SER:HA	18	0.27
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB3	1	0.27
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB2	20	0.27
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD12	10	0.27
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD13	19	0.27
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD12	17	0.27
(2,4192)	1:108:A:VAL:HB	1:103:A:ILE:HD13	2	0.27
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD13	17	0.27
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD12	14	0.27
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD11	1	0.27
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD11	12	0.27
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD12	18	0.27
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD13	2	0.27
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD13	15	0.27
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD11	1	0.27
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD13	18	0.27
(2,4020)	1:49:A:VAL:HB	1:44:A:ILE:HG23	3	0.27
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG23	5	0.27
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG21	9	0.27
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG21	10	0.27
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG23	9	0.27
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG21	20	0.27
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB3	20	0.27
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB1	5	0.27
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB3	18	0.27
(2,3803)	1:42:A:HIS:HB2	1:36:A:LEU:HD23	13	0.27
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG22	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG22	10	0.27
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG23	17	0.27
(2,3705)	1:14:A:PHE:HD2	1:10:A:LEU:HD23	9	0.27
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD22	3	0.27
(2,3684)	1:28:A:LEU:H	1:49:A:VAL:HG21	19	0.27
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG13	20	0.27
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD23	8	0.27
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD22	9	0.27
(2,3670)	1:103:A:ILE:H	1:104:A:LEU:HD22	17	0.27
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG22	13	0.27
(2,3471)	1:118:A:LEU:HA	1:44:A:ILE:HG12	13	0.27
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	6	0.27
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD11	8	0.27
(2,3405)	1:68:A:PHE:HZ	1:118:A:LEU:HD13	12	0.27
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD13	14	0.27
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD22	5	0.27
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	18	0.27
(2,2874)	1:118:A:LEU:HD21	1:48:A:GLU:HG3	2	0.27
(2,2874)	1:118:A:LEU:HD21	1:48:A:GLU:HG3	11	0.27
(2,2845)	1:51:A:LYS:HG2	1:47:A:ASP:HB2	13	0.27
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	8	0.27
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	2	0.27
(2,2538)	1:115:A:TYR:HD2	1:118:A:LEU:HB3	13	0.27
(2,2376)	1:34:A:ILE:HD11	1:42:A:HIS:HA	14	0.27
(2,2318)	1:50:A:GLU:HB2	1:47:A:ASP:HA	13	0.27
(2,2179)	1:108:A:VAL:HG13	1:105:A:ASN:HA	12	0.27
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	9	0.27
(2,2099)	1:131:A:GLU:HG2	1:131:A:GLU:HA	1	0.27
(2,1998)	1:115:A:TYR:HD1	1:112:A:LEU:HA	14	0.27
(2,1998)	1:115:A:TYR:HD1	1:112:A:LEU:HA	16	0.27
(2,1892)	1:8:A:ILE:HG21	1:8:A:ILE:HA	3	0.27
(2,1892)	1:8:A:ILE:HG23	1:8:A:ILE:HA	4	0.27
(2,1891)	1:63:A:LEU:HD21	1:62:A:SER:HB3	6	0.27
(2,1877)	1:137:A:GLU:HB2	1:136:A:SER:HB2	3	0.27
(2,1874)	1:71:A:ILE:HG13	1:82:A:SER:HB3	11	0.27
(2,1781)	1:68:A:PHE:HE1	1:91:A:ILE:HA	2	0.27
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	6	0.27
(2,1601)	1:20:A:GLU:HG3	1:34:A:ILE:H	12	0.27
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	20	0.27
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	18	0.27
(2,1520)	1:25:A:LYS:HB3	1:62:A:SER:H	3	0.27
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1447)	1:22:A:VAL:HG22	1:23:A:THR:H	4	0.27
(2,1447)	1:22:A:VAL:HG21	1:23:A:THR:H	8	0.27
(2,1447)	1:22:A:VAL:HG21	1:23:A:THR:H	19	0.27
(2,1445)	1:65:A:LYS:HG2	1:23:A:THR:H	14	0.27
(2,1440)	1:20:A:GLU:HG2	1:35:A:ARG:HE	19	0.27
(2,1394)	1:64:A:VAL:HG23	1:87:A:ASN:HD22	2	0.27
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	8	0.27
(2,1228)	1:123:A:LEU:HD21	1:124:A:SER:H	16	0.27
(2,1220)	1:99:A:ILE:HG13	1:101:A:ASN:H	3	0.27
(2,1200)	1:36:A:LEU:HB3	1:41:A:TYR:H	19	0.27
(2,1063)	1:23:A:THR:HG23	1:25:A:LYS:H	1	0.27
(2,1063)	1:23:A:THR:HG22	1:25:A:LYS:H	7	0.27
(2,1063)	1:23:A:THR:HG21	1:25:A:LYS:H	13	0.27
(2,1030)	1:22:A:VAL:HB	1:29:A:ASP:H	20	0.27
(2,1027)	1:90:A:ALA:HB3	1:92:A:SER:H	5	0.27
(2,1027)	1:90:A:ALA:HB2	1:92:A:SER:H	6	0.27
(2,1027)	1:90:A:ALA:HB3	1:92:A:SER:H	7	0.27
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	17	0.27
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	18	0.27
(2,895)	1:91:A:ILE:HD13	1:88:A:LYS:H	12	0.27
(2,895)	1:91:A:ILE:HD13	1:88:A:LYS:H	16	0.27
(2,882)	1:28:A:LEU:HD22	1:28:A:LEU:H	4	0.27
(2,882)	1:28:A:LEU:HD22	1:28:A:LEU:H	6	0.27
(2,877)	1:60:A:LEU:HD23	1:86:A:TRP:H	20	0.27
(2,850)	1:139:A:LEU:HD13	1:140:A:GLU:H	15	0.27
(2,848)	1:27:A:ALA:HB1	1:26:A:ASP:H	1	0.27
(2,848)	1:27:A:ALA:HB3	1:26:A:ASP:H	17	0.27
(2,841)	1:139:A:LEU:HD22	1:139:A:LEU:H	17	0.27
(2,831)	1:119:A:ILE:HD12	1:112:A:LEU:H	12	0.27
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	7	0.27
(2,784)	1:61:A:TRP:HB2	1:24:A:ILE:H	6	0.27
(2,605)	1:28:A:LEU:HD23	1:51:A:LYS:H	5	0.27
(2,605)	1:28:A:LEU:HD21	1:51:A:LYS:H	19	0.27
(2,598)	1:24:A:ILE:HG22	1:52:A:LEU:H	3	0.27
(2,597)	1:52:A:LEU:HD13	1:52:A:LEU:H	14	0.27
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	1	0.27
(2,564)	1:104:A:LEU:HD23	1:79:A:TYR:H	8	0.27
(2,564)	1:104:A:LEU:HD22	1:79:A:TYR:H	9	0.27
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	11	0.27
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	20	0.27
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	9	0.27
(2,158)	1:122:A:ILE:HG22	1:123:A:LEU:H	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,156)	1:69:A:ILE:HD11	1:120:A:PHE:H	5	0.27
(2,154)	1:71:A:ILE:HD11	1:122:A:ILE:H	11	0.27
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	10	0.27
(2,65)	1:35:A:ARG:HD2	1:35:A:ARG:H	8	0.27
(2,33)	1:46:A:LYS:HD3	1:46:A:LYS:H	7	0.27
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	10	0.27
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE2	4	0.26
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE2	5	0.26
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE2	7	0.26
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE2	3	0.26
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE2	5	0.26
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE1	6	0.26
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE1	8	0.26
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE1	9	0.26
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE2	13	0.26
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE1	20	0.26
(2,4667)	1:111:A:LEU:HD23	1:115:A:TYR:HE2	11	0.26
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE2	3	0.26
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE2	14	0.26
(2,4551)	1:69:A:ILE:HD12	1:120:A:PHE:HE1	20	0.26
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD1	2	0.26
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD1	20	0.26
(2,4377)	1:112:A:LEU:HD13	1:109:A:GLU:HG3	14	0.26
(2,4373)	1:130:A:THR:HG21	1:134:A:GLU:HB3	20	0.26
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD11	3	0.26
(2,4349)	1:108:A:VAL:HA	1:91:A:ILE:HD12	4	0.26
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD11	8	0.26
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD12	9	0.26
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB1	7	0.26
(2,4310)	1:120:A:PHE:HD2	1:69:A:ILE:HG23	8	0.26
(2,4279)	1:68:A:PHE:HD2	1:118:A:LEU:HD12	6	0.26
(2,4279)	1:68:A:PHE:HD1	1:118:A:LEU:HD12	9	0.26
(2,4236)	1:118:A:LEU:HD23	1:117:A:SER:HA	14	0.26
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD11	7	0.26
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD12	9	0.26
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD11	14	0.26
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD12	15	0.26
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD12	18	0.26
(2,4207)	1:68:A:PHE:HE2	1:91:A:ILE:HD11	9	0.26
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	3	0.26
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	3	0.26
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD13	4	0.26
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD11	6	0.26
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD12	8	0.26
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD13	13	0.26
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD12	17	0.26
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD13	20	0.26
(2,4116)	1:115:A:TYR:HA	1:119:A:ILE:HD12	12	0.26
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	3	0.26
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	13	0.26
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG21	6	0.26
(2,4020)	1:49:A:VAL:HB	1:44:A:ILE:HG21	6	0.26
(2,4020)	1:118:A:LEU:HB3	1:44:A:ILE:HG23	10	0.26
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG23	17	0.26
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG23	20	0.26
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG23	7	0.26
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG21	11	0.26
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB1	7	0.26
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG11	2	0.26
(2,3826)	1:79:A:TYR:HB2	1:108:A:VAL:HG13	5	0.26
(2,3826)	1:109:A:GLU:HG3	1:108:A:VAL:HG12	20	0.26
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG23	14	0.26
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	2	0.26
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	2	0.26
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	2	0.26
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG12	3	0.26
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG13	3	0.26
(2,3635)	1:52:A:LEU:HD13	1:56:A:ILE:HG12	5	0.26
(2,3635)	1:52:A:LEU:HD12	1:56:A:ILE:HG12	16	0.26
(2,3632)	1:94:A:LEU:HD11	1:95:A:LEU:HG	5	0.26
(2,3632)	1:94:A:LEU:HD12	1:95:A:LEU:HG	13	0.26
(2,3405)	1:115:A:TYR:HE2	1:118:A:LEU:HD11	1	0.26
(2,3389)	1:21:A:TYR:HD1	1:69:A:ILE:HG13	20	0.26
(2,3361)	1:87:A:ASN:HD22	1:64:A:VAL:HG22	8	0.26
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	3	0.26
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	4	0.26
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD11	1	0.26
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD12	5	0.26
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD21	15	0.26
(2,3271)	1:28:A:LEU:HD12	1:25:A:LYS:HD3	16	0.26
(2,3247)	1:60:A:LEU:HD23	1:89:A:LYS:HB3	4	0.26
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	10	0.26
(2,3017)	1:66:A:ILE:H	1:65:A:LYS:HD3	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3009)	1:34:A:ILE:HG22	1:20:A:GLU:HG2	8	0.26
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	10	0.26
(2,2955)	1:75:A:GLU:HA	1:75:A:GLU:HG2	8	0.26
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	19	0.26
(2,2658)	1:81:A:VAL:HG22	1:79:A:TYR:HB2	2	0.26
(2,2658)	1:81:A:VAL:HG21	1:79:A:TYR:HB2	16	0.26
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	20	0.26
(2,2494)	1:10:A:LEU:HB2	1:9:A:GLY:HA2	5	0.26
(2,2473)	1:69:A:ILE:HD11	1:18:A:PRO:HD3	8	0.26
(2,2473)	1:69:A:ILE:HD12	1:18:A:PRO:HD3	9	0.26
(2,2376)	1:34:A:ILE:HD13	1:42:A:HIS:HA	3	0.26
(2,2364)	1:93:A:ILE:HG21	1:90:A:ALA:HA	8	0.26
(2,2174)	1:99:A:ILE:HD12	1:89:A:LYS:HA	11	0.26
(2,2143)	1:133:A:THR:HG22	1:134:A:GLU:HA	2	0.26
(2,2143)	1:133:A:THR:HG22	1:134:A:GLU:HA	14	0.26
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	14	0.26
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	9	0.26
(2,1990)	1:68:A:PHE:HD2	1:66:A:ILE:HA	20	0.26
(2,1904)	1:56:A:ILE:HD13	1:53:A:SER:HA	18	0.26
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	2	0.26
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	11	0.26
(2,1660)	1:130:A:THR:HG22	1:132:A:GLU:H	11	0.26
(2,1632)	1:134:A:GLU:HB3	1:136:A:SER:H	20	0.26
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	8	0.26
(2,1567)	1:32:A:LEU:HA	1:27:A:ALA:H	14	0.26
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	8	0.26
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	12	0.26
(2,1541)	1:22:A:VAL:HB	1:30:A:GLY:H	1	0.26
(2,1540)	1:31:A:LYS:HB3	1:30:A:GLY:H	17	0.26
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	11	0.26
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	15	0.26
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	5	0.26
(2,1447)	1:22:A:VAL:HG23	1:23:A:THR:H	2	0.26
(2,1447)	1:22:A:VAL:HG21	1:23:A:THR:H	3	0.26
(2,1447)	1:22:A:VAL:HG22	1:23:A:THR:H	6	0.26
(2,1447)	1:22:A:VAL:HG22	1:23:A:THR:H	10	0.26
(2,1386)	1:65:A:LYS:HD3	1:21:A:TYR:H	15	0.26
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	1	0.26
(2,1255)	1:52:A:LEU:HD12	1:54:A:SER:H	9	0.26
(2,1255)	1:52:A:LEU:HD11	1:54:A:SER:H	11	0.26
(2,1248)	1:94:A:LEU:HD11	1:95:A:LEU:H	10	0.26
(2,1236)	1:36:A:LEU:HD13	1:38:A:ASN:H	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	3	0.26
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	9	0.26
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	6	0.26
(2,1082)	1:24:A:ILE:HG23	1:25:A:LYS:H	1	0.26
(2,1063)	1:23:A:THR:HG23	1:25:A:LYS:H	8	0.26
(2,1063)	1:23:A:THR:HG21	1:25:A:LYS:H	10	0.26
(2,1063)	1:23:A:THR:HG21	1:25:A:LYS:H	18	0.26
(2,1063)	1:23:A:THR:HG23	1:25:A:LYS:H	19	0.26
(2,1027)	1:90:A:ALA:HB2	1:92:A:SER:H	1	0.26
(2,1027)	1:90:A:ALA:HB2	1:92:A:SER:H	15	0.26
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	8	0.26
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	9	0.26
(2,895)	1:91:A:ILE:HD11	1:88:A:LYS:H	18	0.26
(2,886)	1:28:A:LEU:HD11	1:26:A:ASP:H	3	0.26
(2,885)	1:66:A:ILE:HD11	1:26:A:ASP:H	6	0.26
(2,877)	1:60:A:LEU:HD21	1:86:A:TRP:H	1	0.26
(2,850)	1:139:A:LEU:HD13	1:140:A:GLU:H	17	0.26
(2,831)	1:119:A:ILE:HD13	1:112:A:LEU:H	19	0.26
(2,784)	1:61:A:TRP:HB2	1:24:A:ILE:H	13	0.26
(2,764)	1:29:A:ASP:HB3	1:28:A:LEU:H	4	0.26
(2,764)	1:29:A:ASP:HB3	1:28:A:LEU:H	9	0.26
(2,597)	1:52:A:LEU:HD11	1:52:A:LEU:H	1	0.26
(2,597)	1:52:A:LEU:HD12	1:52:A:LEU:H	5	0.26
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	18	0.26
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	2	0.26
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	18	0.26
(2,571)	1:118:A:LEU:HD12	1:52:A:LEU:H	12	0.26
(2,564)	1:104:A:LEU:HD12	1:79:A:TYR:H	17	0.26
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	10	0.26
(2,348)	1:58:A:LEU:HD22	1:61:A:TRP:H	11	0.26
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	9	0.26
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	9	0.26
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	9	0.26
(2,161)	1:69:A:ILE:HG21	1:70:A:PHE:H	7	0.26
(2,154)	1:71:A:ILE:HD12	1:122:A:ILE:H	4	0.26
(2,33)	1:46:A:LYS:HD2	1:46:A:LYS:H	20	0.26
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	14	0.26
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE1	1	0.25
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE2	2	0.25
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE2	3	0.25
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE1	8	0.25
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE1	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE1	20	0.25
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE2	4	0.25
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE2	2	0.25
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE1	8	0.25
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE1	11	0.25
(2,4474)	1:36:A:LEU:HD21	1:41:A:TYR:HD1	6	0.25
(2,4474)	1:36:A:LEU:HD22	1:41:A:TYR:HD2	8	0.25
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	2	0.25
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	5	0.25
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	9	0.25
(2,4334)	1:120:A:PHE:HB2	1:69:A:ILE:HD13	8	0.25
(2,4310)	1:120:A:PHE:HD1	1:69:A:ILE:HG21	19	0.25
(2,4303)	1:89:A:LYS:HD2	1:63:A:LEU:HD11	6	0.25
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD13	6	0.25
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD11	15	0.25
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD11	11	0.25
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD12	17	0.25
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD13	20	0.25
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD13	7	0.25
(2,4136)	1:76:A:ILE:HA	1:76:A:ILE:HD13	12	0.25
(2,4105)	1:59:A:TYR:HE2	1:93:A:ILE:HD11	16	0.25
(2,4095)	1:25:A:LYS:H	1:66:A:ILE:HD13	17	0.25
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD13	10	0.25
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	17	0.25
(2,4020)	1:67:A:PRO:HB3	1:44:A:ILE:HG23	17	0.25
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG23	14	0.25
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG21	7	0.25
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG22	18	0.25
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG21	10	0.25
(2,3838)	1:31:A:LYS:HG3	1:22:A:VAL:HG12	15	0.25
(2,3826)	1:79:A:TYR:HB2	1:108:A:VAL:HG11	7	0.25
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG11	7	0.25
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG12	7	0.25
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG13	7	0.25
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG11	7	0.25
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG12	8	0.25
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG13	15	0.25
(2,3601)	1:56:A:ILE:HB	1:52:A:LEU:HD11	10	0.25
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	4	0.25
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	8	0.25
(2,3389)	1:41:A:TYR:HD1	1:36:A:LEU:HG	10	0.25
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD13	6	0.25
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD11	16	0.25
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD12	20	0.25
(2,3085)	1:21:A:TYR:HD1	1:20:A:GLU:HB2	11	0.25
(2,3065)	1:70:A:PHE:HD1	1:81:A:VAL:HB	9	0.25
(2,3017)	1:66:A:ILE:H	1:65:A:LYS:HD3	5	0.25
(2,3017)	1:104:A:LEU:H	1:97:A:ARG:HG3	8	0.25
(2,2827)	1:45:A:LYS:HB3	1:47:A:ASP:HB3	6	0.25
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	14	0.25
(2,2796)	1:76:A:ILE:HA	1:76:A:ILE:HB	8	0.25
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	20	0.25
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	11	0.25
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	16	0.25
(2,2542)	1:115:A:TYR:HD2	1:111:A:LEU:HB2	18	0.25
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	11	0.25
(2,2375)	1:104:A:LEU:HD22	1:78:A:GLU:HA	14	0.25
(2,2194)	1:28:A:LEU:HD12	1:54:A:SER:HA	14	0.25
(2,2179)	1:108:A:VAL:HG11	1:105:A:ASN:HA	4	0.25
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	7	0.25
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	12	0.25
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	16	0.25
(2,2099)	1:131:A:GLU:HG2	1:131:A:GLU:HA	11	0.25
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	11	0.25
(2,1904)	1:56:A:ILE:HD12	1:53:A:SER:HA	20	0.25
(2,1894)	1:76:A:ILE:HD13	1:76:A:ILE:HA	12	0.25
(2,1891)	1:63:A:LEU:HD22	1:62:A:SER:HB3	5	0.25
(2,1866)	1:139:A:LEU:HB2	1:136:A:SER:HB3	1	0.25
(2,1866)	1:139:A:LEU:HB2	1:136:A:SER:HB3	5	0.25
(2,1839)	1:76:A:ILE:HB	1:76:A:ILE:HA	8	0.25
(2,1686)	1:24:A:ILE:HG21	1:23:A:THR:HB	19	0.25
(2,1599)	1:62:A:SER:HA	1:26:A:ASP:H	16	0.25
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	9	0.25
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	10	0.25
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	12	0.25
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	20	0.25
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	5	0.25
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	10	0.25
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	16	0.25
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	19	0.25
(2,1540)	1:31:A:LYS:HB3	1:30:A:GLY:H	5	0.25
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	7	0.25
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	7	0.25
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	12	0.25
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	11	0.25
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	15	0.25
(2,1447)	1:22:A:VAL:HG22	1:23:A:THR:H	11	0.25
(2,1447)	1:22:A:VAL:HG22	1:23:A:THR:H	12	0.25
(2,1447)	1:22:A:VAL:HG21	1:23:A:THR:H	14	0.25
(2,1447)	1:22:A:VAL:HG22	1:23:A:THR:H	15	0.25
(2,1447)	1:22:A:VAL:HG23	1:23:A:THR:H	18	0.25
(2,1445)	1:65:A:LYS:HG2	1:23:A:THR:H	10	0.25
(2,1440)	1:20:A:GLU:HG2	1:35:A:ARG:HE	20	0.25
(2,1404)	1:69:A:ILE:HD11	1:37:A:ASN:HD22	8	0.25
(2,1388)	1:22:A:VAL:HG12	1:21:A:TYR:H	7	0.25
(2,1248)	1:94:A:LEU:HD12	1:95:A:LEU:H	8	0.25
(2,1248)	1:94:A:LEU:HD13	1:95:A:LEU:H	11	0.25
(2,1248)	1:94:A:LEU:HD12	1:95:A:LEU:H	16	0.25
(2,1236)	1:19:A:ALA:HB3	1:38:A:ASN:H	12	0.25
(2,1219)	1:46:A:LYS:HG2	1:47:A:ASP:H	12	0.25
(2,1200)	1:36:A:LEU:HB3	1:41:A:TYR:H	15	0.25
(2,1199)	1:102:A:VAL:HB	1:101:A:ASN:H	5	0.25
(2,1166)	1:124:A:SER:HB3	1:124:A:SER:H	9	0.25
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	13	0.25
(2,1082)	1:24:A:ILE:HG23	1:25:A:LYS:H	18	0.25
(2,1063)	1:23:A:THR:HG22	1:25:A:LYS:H	12	0.25
(2,1030)	1:22:A:VAL:HB	1:29:A:ASP:H	7	0.25
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	3	0.25
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	5	0.25
(2,1016)	1:45:A:LYS:HB3	1:117:A:SER:H	13	0.25
(2,962)	1:95:A:LEU:HA	1:97:A:ARG:H	14	0.25
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	9	0.25
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	15	0.25
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	18	0.25
(2,874)	1:49:A:VAL:HG22	1:48:A:GLU:H	4	0.25
(2,871)	1:119:A:ILE:HD12	1:119:A:ILE:H	17	0.25
(2,850)	1:139:A:LEU:HD11	1:140:A:GLU:H	5	0.25
(2,841)	1:139:A:LEU:HD23	1:139:A:LEU:H	6	0.25
(2,831)	1:112:A:LEU:HD21	1:112:A:LEU:H	7	0.25
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	9	0.25
(2,791)	1:111:A:LEU:HB3	1:112:A:LEU:H	12	0.25
(2,784)	1:61:A:TRP:HB2	1:24:A:ILE:H	11	0.25
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	9	0.25
(2,597)	1:52:A:LEU:HD13	1:52:A:LEU:H	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,597)	1:52:A:LEU:HD11	1:52:A:LEU:H	16	0.25
(2,597)	1:52:A:LEU:HD12	1:52:A:LEU:H	20	0.25
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	7	0.25
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	17	0.25
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	16	0.25
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	7	0.25
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	16	0.25
(2,253)	1:22:A:VAL:HG21	1:27:A:ALA:H	8	0.25
(2,225)	1:98:A:GLU:HG2	1:99:A:ILE:H	9	0.25
(2,160)	1:121:A:ILE:HG22	1:70:A:PHE:H	18	0.25
(2,154)	1:71:A:ILE:HD11	1:122:A:ILE:H	3	0.25
(2,145)	1:122:A:ILE:HG13	1:70:A:PHE:H	2	0.25
(2,145)	1:122:A:ILE:HG13	1:70:A:PHE:H	6	0.25
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	2	0.25
(2,108)	1:67:A:PRO:HA	1:120:A:PHE:H	7	0.25
(2,80)	1:34:A:ILE:HG22	1:35:A:ARG:H	8	0.25
(2,34)	1:71:A:ILE:HG21	1:72:A:LYS:H	1	0.25
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	19	0.25
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE1	9	0.24
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE2	14	0.24
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE1	18	0.24
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE2	2	0.24
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE2	10	0.24
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE2	17	0.24
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE1	18	0.24
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE1	19	0.24
(2,4505)	1:122:A:ILE:HD13	1:14:A:PHE:HD2	6	0.24
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	19	0.24
(2,4465)	1:118:A:LEU:HD11	1:115:A:TYR:HD1	2	0.24
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD2	17	0.24
(2,4385)	1:46:A:LYS:HE2	1:50:A:GLU:HG2	12	0.24
(2,4377)	1:135:A:LEU:HD22	1:134:A:GLU:HG3	13	0.24
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB3	16	0.24
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB2	11	0.24
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD11	5	0.24
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD13	8	0.24
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD13	13	0.24
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD12	17	0.24
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD13	20	0.24
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD11	4	0.24
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD13	4	0.24
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD12	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	14	0.24
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	14	0.24
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	14	0.24
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD13	11	0.24
(2,4092)	1:14:A:PHE:HD2	1:122:A:ILE:HD13	6	0.24
(2,4077)	1:90:A:ALA:H	1:56:A:ILE:HD12	8	0.24
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	12	0.24
(2,4020)	1:118:A:LEU:HB3	1:44:A:ILE:HG23	18	0.24
(2,4020)	1:49:A:VAL:HB	1:44:A:ILE:HG21	20	0.24
(2,4012)	1:68:A:PHE:HB3	1:66:A:ILE:HG23	9	0.24
(2,4006)	1:80:A:PHE:HB3	1:99:A:ILE:HG21	1	0.24
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG23	11	0.24
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG23	9	0.24
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB3	6	0.24
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB2	14	0.24
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	3	0.24
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	3	0.24
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	3	0.24
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD21	15	0.24
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG21	18	0.24
(2,3559)	1:115:A:TYR:HB2	1:118:A:LEU:HD21	12	0.24
(2,3343)	1:86:A:TRP:HZ3	1:89:A:LYS:HG3	17	0.24
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD23	2	0.24
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD11	4	0.24
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD11	11	0.24
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD13	13	0.24
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD22	15	0.24
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD11	19	0.24
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	15	0.24
(2,3050)	1:143:A:HIS:HD2	1:143:A:HIS:HB3	14	0.24
(2,2954)	1:137:A:GLU:HA	1:137:A:GLU:HG2	1	0.24
(2,2954)	1:137:A:GLU:HA	1:137:A:GLU:HG2	18	0.24
(2,2844)	1:51:A:LYS:HD2	1:47:A:ASP:HB3	14	0.24
(2,2827)	1:50:A:GLU:HB2	1:47:A:ASP:HB3	4	0.24
(2,2827)	1:50:A:GLU:HB2	1:47:A:ASP:HB3	8	0.24
(2,2827)	1:45:A:LYS:HB3	1:47:A:ASP:HB3	19	0.24
(2,2806)	1:15:A:SER:HB2	1:38:A:ASN:HB2	5	0.24
(2,2806)	1:15:A:SER:HB3	1:38:A:ASN:HB2	13	0.24
(2,2806)	1:15:A:SER:HB2	1:38:A:ASN:HB2	17	0.24
(2,2796)	1:76:A:ILE:HA	1:76:A:ILE:HB	1	0.24
(2,2796)	1:76:A:ILE:HA	1:76:A:ILE:HB	4	0.24
(2,2796)	1:76:A:ILE:HA	1:76:A:ILE:HB	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2796)	1:5:A:ILE:HA	1:5:A:ILE:HB	6	0.24
(2,2796)	1:5:A:ILE:HA	1:5:A:ILE:HB	7	0.24
(2,2796)	1:5:A:ILE:HA	1:5:A:ILE:HB	9	0.24
(2,2796)	1:76:A:ILE:HA	1:76:A:ILE:HB	10	0.24
(2,2796)	1:76:A:ILE:HA	1:76:A:ILE:HB	14	0.24
(2,2796)	1:76:A:ILE:HA	1:76:A:ILE:HB	15	0.24
(2,2796)	1:5:A:ILE:HA	1:5:A:ILE:HB	17	0.24
(2,2796)	1:5:A:ILE:HA	1:5:A:ILE:HB	18	0.24
(2,2796)	1:5:A:ILE:HA	1:5:A:ILE:HB	19	0.24
(2,2653)	1:95:A:LEU:HD11	1:107:A:ASP:HB2	15	0.24
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	7	0.24
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	15	0.24
(2,2372)	1:34:A:ILE:HG21	1:21:A:TYR:HA	11	0.24
(2,2340)	1:114:A:GLU:HB3	1:115:A:TYR:HA	6	0.24
(2,2143)	1:133:A:THR:HG23	1:134:A:GLU:HA	4	0.24
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	9	0.24
(2,2099)	1:134:A:GLU:HG2	1:134:A:GLU:HA	18	0.24
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	2	0.24
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	6	0.24
(2,1998)	1:115:A:TYR:HD1	1:112:A:LEU:HA	3	0.24
(2,1904)	1:56:A:ILE:HD13	1:53:A:SER:HA	14	0.24
(2,1891)	1:63:A:LEU:HD22	1:62:A:SER:HB3	8	0.24
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	8	0.24
(2,1839)	1:76:A:ILE:HB	1:76:A:ILE:HA	1	0.24
(2,1839)	1:76:A:ILE:HB	1:76:A:ILE:HA	4	0.24
(2,1839)	1:76:A:ILE:HB	1:76:A:ILE:HA	5	0.24
(2,1839)	1:5:A:ILE:HB	1:5:A:ILE:HA	6	0.24
(2,1839)	1:5:A:ILE:HB	1:5:A:ILE:HA	7	0.24
(2,1839)	1:5:A:ILE:HB	1:5:A:ILE:HA	9	0.24
(2,1839)	1:76:A:ILE:HB	1:76:A:ILE:HA	10	0.24
(2,1839)	1:76:A:ILE:HB	1:76:A:ILE:HA	14	0.24
(2,1839)	1:76:A:ILE:HB	1:76:A:ILE:HA	15	0.24
(2,1839)	1:5:A:ILE:HB	1:5:A:ILE:HA	17	0.24
(2,1839)	1:5:A:ILE:HB	1:5:A:ILE:HA	18	0.24
(2,1839)	1:5:A:ILE:HB	1:5:A:ILE:HA	19	0.24
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB2	5	0.24
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB3	13	0.24
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB2	17	0.24
(2,1731)	1:56:A:ILE:HG22	1:24:A:ILE:HA	19	0.24
(2,1718)	1:64:A:VAL:HB	1:24:A:ILE:HA	5	0.24
(2,1660)	1:130:A:THR:HG21	1:132:A:GLU:H	1	0.24
(2,1660)	1:130:A:THR:HG23	1:132:A:GLU:H	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	8	0.24
(2,1626)	1:139:A:LEU:HD12	1:136:A:SER:H	8	0.24
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	13	0.24
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	14	0.24
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	7	0.24
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	19	0.24
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	1	0.24
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	4	0.24
(2,1542)	1:46:A:LYS:HG3	1:30:A:GLY:H	13	0.24
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	19	0.24
(2,1540)	1:31:A:LYS:HB3	1:30:A:GLY:H	20	0.24
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	4	0.24
(2,1499)	1:93:A:ILE:HG22	1:96:A:GLY:H	5	0.24
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	8	0.24
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	18	0.24
(2,1447)	1:22:A:VAL:HG21	1:23:A:THR:H	9	0.24
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	11	0.24
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	16	0.24
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	16	0.24
(2,1255)	1:52:A:LEU:HD12	1:54:A:SER:H	8	0.24
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	15	0.24
(2,1234)	1:94:A:LEU:HD23	1:56:A:ILE:H	13	0.24
(2,1220)	1:99:A:ILE:HG13	1:101:A:ASN:H	2	0.24
(2,1200)	1:43:A:GLU:HG3	1:41:A:TYR:H	1	0.24
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	5	0.24
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	16	0.24
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	11	0.24
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	15	0.24
(2,1063)	1:23:A:THR:HG22	1:25:A:LYS:H	14	0.24
(2,1063)	1:23:A:THR:HG23	1:25:A:LYS:H	16	0.24
(2,1063)	1:23:A:THR:HG23	1:25:A:LYS:H	17	0.24
(2,1056)	1:91:A:ILE:HG22	1:92:A:SER:H	10	0.24
(2,1027)	1:90:A:ALA:HB1	1:92:A:SER:H	17	0.24
(2,1027)	1:90:A:ALA:HB3	1:92:A:SER:H	20	0.24
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	3	0.24
(2,910)	1:27:A:ALA:H	1:29:A:ASP:H	4	0.24
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	5	0.24
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	12	0.24
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	17	0.24
(2,885)	1:66:A:ILE:HD13	1:26:A:ASP:H	14	0.24
(2,848)	1:27:A:ALA:HB2	1:26:A:ASP:H	15	0.24
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,819)	1:112:A:LEU:HB2	1:111:A:LEU:H	2	0.24
(2,816)	1:52:A:LEU:HB2	1:49:A:VAL:H	7	0.24
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	12	0.24
(2,760)	1:41:A:TYR:HB2	1:34:A:ILE:H	16	0.24
(2,605)	1:28:A:LEU:HD23	1:51:A:LYS:H	1	0.24
(2,598)	1:24:A:ILE:HG23	1:52:A:LEU:H	6	0.24
(2,597)	1:52:A:LEU:HD23	1:52:A:LEU:H	2	0.24
(2,597)	1:52:A:LEU:HD11	1:52:A:LEU:H	4	0.24
(2,597)	1:52:A:LEU:HD11	1:52:A:LEU:H	11	0.24
(2,597)	1:52:A:LEU:HD13	1:52:A:LEU:H	13	0.24
(2,597)	1:52:A:LEU:HD22	1:52:A:LEU:H	15	0.24
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	8	0.24
(2,560)	1:95:A:LEU:HD11	1:104:A:LEU:H	1	0.24
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	9	0.24
(2,532)	1:51:A:LYS:HB2	1:52:A:LEU:H	15	0.24
(2,527)	1:72:A:LYS:HD3	1:79:A:TYR:H	9	0.24
(2,516)	1:72:A:LYS:HD2	1:80:A:PHE:H	15	0.24
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	19	0.24
(2,401)	1:70:A:PHE:HE1	1:69:A:ILE:H	13	0.24
(2,396)	1:21:A:TYR:HE2	1:68:A:PHE:H	9	0.24
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	11	0.24
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	15	0.24
(2,225)	1:98:A:GLU:HG2	1:99:A:ILE:H	13	0.24
(2,158)	1:122:A:ILE:HG22	1:123:A:LEU:H	4	0.24
(2,154)	1:71:A:ILE:HD11	1:122:A:ILE:H	16	0.24
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	15	0.24
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	3	0.24
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	13	0.24
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	9	0.24
(2,95)	1:70:A:PHE:HD1	1:122:A:ILE:H	5	0.24
(2,84)	1:24:A:ILE:HG23	1:61:A:TRP:HE1	4	0.24
(2,84)	1:24:A:ILE:HG22	1:61:A:TRP:HE1	6	0.24
(2,34)	1:71:A:ILE:HG22	1:72:A:LYS:H	5	0.24
(2,34)	1:71:A:ILE:HG21	1:72:A:LYS:H	14	0.24
(2,33)	1:46:A:LYS:HD2	1:46:A:LYS:H	2	0.24
(2,4709)	1:57:A:PRO:HD3	1:59:A:TYR:HE2	16	0.23
(2,4689)	1:123:A:LEU:HD22	1:79:A:TYR:HD2	12	0.23
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE2	2	0.23
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE2	10	0.23
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE1	1	0.23
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE1	13	0.23
(2,4570)	1:60:A:LEU:HD22	1:86:A:TRP:HD1	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4474)	1:36:A:LEU:HD21	1:41:A:TYR:HD1	13	0.23
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	6	0.23
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	15	0.23
(2,4398)	1:113:A:ARG:HA	1:113:A:ARG:HD3	12	0.23
(2,4372)	1:60:A:LEU:HD23	1:86:A:TRP:HB2	6	0.23
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB3	6	0.23
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD12	1	0.23
(2,4214)	1:91:A:ILE:HB	1:91:A:ILE:HD13	11	0.23
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD11	16	0.23
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD13	2	0.23
(2,4120)	1:21:A:TYR:HA	1:44:A:ILE:HD11	9	0.23
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG21	6	0.23
(2,4093)	1:120:A:PHE:HD2	1:122:A:ILE:HD13	15	0.23
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD11	2	0.23
(2,4026)	1:118:A:LEU:HB2	1:66:A:ILE:HG22	6	0.23
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG22	4	0.23
(2,4020)	1:118:A:LEU:HB3	1:44:A:ILE:HG23	9	0.23
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG23	15	0.23
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG22	1	0.23
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG22	18	0.23
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG21	19	0.23
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG21	20	0.23
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG22	13	0.23
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB1	11	0.23
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG11	16	0.23
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG12	16	0.23
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG13	16	0.23
(2,3714)	1:49:A:VAL:H	1:28:A:LEU:HD21	11	0.23
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD23	4	0.23
(2,3685)	1:121:A:ILE:H	1:112:A:LEU:HD21	9	0.23
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG12	11	0.23
(2,3601)	1:56:A:ILE:HB	1:52:A:LEU:HD11	2	0.23
(2,3471)	1:32:A:LEU:HA	1:44:A:ILE:HG13	17	0.23
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	5	0.23
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	13	0.23
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	16	0.23
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD11	3	0.23
(2,3409)	1:79:A:TYR:HD2	1:123:A:LEU:HD21	14	0.23
(2,3389)	1:21:A:TYR:HD1	1:69:A:ILE:HG13	7	0.23
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD11	10	0.23
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD11	17	0.23
(2,3247)	1:60:A:LEU:HD23	1:89:A:LYS:HB3	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3085)	1:21:A:TYR:HD1	1:20:A:GLU:HB2	2	0.23
(2,2955)	1:75:A:GLU:HA	1:75:A:GLU:HG2	7	0.23
(2,2954)	1:132:A:GLU:HA	1:132:A:GLU:HG2	20	0.23
(2,2827)	1:45:A:LYS:HB3	1:47:A:ASP:HB3	20	0.23
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	20	0.23
(2,2796)	1:76:A:ILE:HA	1:76:A:ILE:HB	2	0.23
(2,2796)	1:5:A:ILE:HA	1:5:A:ILE:HB	3	0.23
(2,2796)	1:5:A:ILE:HA	1:5:A:ILE:HB	11	0.23
(2,2796)	1:5:A:ILE:HA	1:5:A:ILE:HB	12	0.23
(2,2796)	1:76:A:ILE:HA	1:76:A:ILE:HB	13	0.23
(2,2796)	1:76:A:ILE:HA	1:76:A:ILE:HB	16	0.23
(2,2796)	1:5:A:ILE:HA	1:5:A:ILE:HB	20	0.23
(2,2658)	1:81:A:VAL:HG21	1:79:A:TYR:HB2	5	0.23
(2,2658)	1:81:A:VAL:HG23	1:79:A:TYR:HB2	18	0.23
(2,2560)	1:42:A:HIS:HD2	1:34:A:ILE:HB	9	0.23
(2,2490)	1:31:A:LYS:HG2	1:30:A:GLY:HA3	19	0.23
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	5	0.23
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	14	0.23
(2,2377)	1:52:A:LEU:HD21	1:115:A:TYR:HA	7	0.23
(2,2376)	1:34:A:ILE:HD11	1:42:A:HIS:HA	17	0.23
(2,2375)	1:104:A:LEU:HD23	1:78:A:GLU:HA	2	0.23
(2,2338)	1:72:A:LYS:HD3	1:79:A:TYR:HA	20	0.23
(2,2179)	1:108:A:VAL:HG13	1:105:A:ASN:HA	2	0.23
(2,2163)	1:102:A:VAL:HG21	1:103:A:ILE:HA	20	0.23
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	6	0.23
(2,1948)	1:92:A:SER:H	1:99:A:ILE:HA	17	0.23
(2,1891)	1:63:A:LEU:HD21	1:62:A:SER:HB3	7	0.23
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	6	0.23
(2,1839)	1:76:A:ILE:HB	1:76:A:ILE:HA	2	0.23
(2,1839)	1:5:A:ILE:HB	1:5:A:ILE:HA	3	0.23
(2,1839)	1:5:A:ILE:HB	1:5:A:ILE:HA	11	0.23
(2,1839)	1:5:A:ILE:HB	1:5:A:ILE:HA	12	0.23
(2,1839)	1:76:A:ILE:HB	1:76:A:ILE:HA	13	0.23
(2,1839)	1:76:A:ILE:HB	1:76:A:ILE:HA	16	0.23
(2,1839)	1:5:A:ILE:HB	1:5:A:ILE:HA	20	0.23
(2,1833)	1:51:A:LYS:HB2	1:54:A:SER:HB2	20	0.23
(2,1654)	1:41:A:TYR:HB3	1:36:A:LEU:H	14	0.23
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	19	0.23
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	2	0.23
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	11	0.23
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	4	0.23
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	10	0.23
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	9	0.23
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	14	0.23
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	17	0.23
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	19	0.23
(2,1394)	1:64:A:VAL:HG23	1:87:A:ASN:HD22	14	0.23
(2,1321)	1:113:A:ARG:HD2	1:114:A:GLU:H	6	0.23
(2,1273)	1:115:A:TYR:HD2	1:53:A:SER:H	9	0.23
(2,1256)	1:28:A:LEU:HD12	1:54:A:SER:H	14	0.23
(2,1255)	1:52:A:LEU:HD11	1:54:A:SER:H	15	0.23
(2,1248)	1:94:A:LEU:HD11	1:95:A:LEU:H	2	0.23
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	17	0.23
(2,1188)	1:37:A:ASN:HB3	1:15:A:SER:H	20	0.23
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	9	0.23
(2,1104)	1:37:A:ASN:H	1:20:A:GLU:H	11	0.23
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	19	0.23
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	12	0.23
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	15	0.23
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	8	0.23
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	16	0.23
(2,895)	1:91:A:ILE:HD13	1:88:A:LYS:H	15	0.23
(2,885)	1:66:A:ILE:HD12	1:26:A:ASP:H	16	0.23
(2,882)	1:28:A:LEU:HD23	1:28:A:LEU:H	9	0.23
(2,874)	1:49:A:VAL:HG23	1:48:A:GLU:H	15	0.23
(2,862)	1:111:A:LEU:HD23	1:111:A:LEU:H	15	0.23
(2,850)	1:139:A:LEU:HD13	1:140:A:GLU:H	7	0.23
(2,850)	1:139:A:LEU:HD13	1:140:A:GLU:H	16	0.23
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	14	0.23
(2,819)	1:110:A:LYS:HD3	1:111:A:LEU:H	9	0.23
(2,816)	1:51:A:LYS:HG2	1:49:A:VAL:H	6	0.23
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	13	0.23
(2,663)	1:115:A:TYR:HD2	1:112:A:LEU:H	7	0.23
(2,605)	1:28:A:LEU:HD22	1:51:A:LYS:H	17	0.23
(2,597)	1:52:A:LEU:HD11	1:52:A:LEU:H	10	0.23
(2,597)	1:52:A:LEU:HD11	1:52:A:LEU:H	17	0.23
(2,582)	1:56:A:ILE:HG13	1:55:A:ARG:H	17	0.23
(2,527)	1:72:A:LYS:HD3	1:79:A:TYR:H	14	0.23
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	13	0.23
(2,510)	1:65:A:LYS:HE2	1:64:A:VAL:H	7	0.23
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	5	0.23
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	13	0.23
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	1	0.23
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	1	0.23
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	1	0.23
(2,166)	1:22:A:VAL:HG11	1:31:A:LYS:H	12	0.23
(2,166)	1:22:A:VAL:HG12	1:31:A:LYS:H	12	0.23
(2,166)	1:22:A:VAL:HG13	1:31:A:LYS:H	12	0.23
(2,158)	1:122:A:ILE:HG21	1:123:A:LEU:H	9	0.23
(2,158)	1:122:A:ILE:HG23	1:123:A:LEU:H	10	0.23
(2,145)	1:122:A:ILE:HG13	1:70:A:PHE:H	17	0.23
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	6	0.23
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	14	0.23
(2,118)	1:125:A:PRO:HD3	1:123:A:LEU:H	19	0.23
(2,95)	1:70:A:PHE:HD1	1:122:A:ILE:H	15	0.23
(2,84)	1:24:A:ILE:HG21	1:61:A:TRP:HE1	15	0.23
(2,34)	1:71:A:ILE:HG22	1:72:A:LYS:H	8	0.23
(2,34)	1:71:A:ILE:HG21	1:72:A:LYS:H	17	0.23
(2,34)	1:71:A:ILE:HG23	1:72:A:LYS:H	19	0.23
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE1	1	0.22
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE1	12	0.22
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE2	14	0.22
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE1	20	0.22
(2,4641)	1:115:A:TYR:HA	1:115:A:TYR:HE2	9	0.22
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	5	0.22
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD2	19	0.22
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	7	0.22
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	20	0.22
(2,4385)	1:129:A:TYR:HB3	1:131:A:GLU:HG3	16	0.22
(2,4320)	1:24:A:ILE:HB	1:66:A:ILE:HG22	9	0.22
(2,4320)	1:24:A:ILE:HB	1:66:A:ILE:HG22	12	0.22
(2,4236)	1:118:A:LEU:HD22	1:117:A:SER:HA	9	0.22
(2,4225)	1:23:A:THR:HG23	1:62:A:SER:HB2	19	0.22
(2,4207)	1:70:A:PHE:HE1	1:91:A:ILE:HD12	12	0.22
(2,4207)	1:70:A:PHE:HE2	1:91:A:ILE:HD11	20	0.22
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD11	7	0.22
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD12	10	0.22
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD13	12	0.22
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD11	19	0.22
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG23	18	0.22
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD11	18	0.22
(2,4020)	1:118:A:LEU:HB3	1:44:A:ILE:HG23	2	0.22
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG21	6	0.22
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG22	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB3	13	0.22
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG22	15	0.22
(2,3811)	1:48:A:GLU:HB2	1:49:A:VAL:HG23	13	0.22
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD23	2	0.22
(2,3632)	1:94:A:LEU:HD11	1:95:A:LEU:HG	2	0.22
(2,3471)	1:32:A:LEU:HA	1:44:A:ILE:HG13	18	0.22
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	8	0.22
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	19	0.22
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD13	18	0.22
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD12	8	0.22
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD21	11	0.22
(2,3300)	1:68:A:PHE:H	1:118:A:LEU:HD11	15	0.22
(2,3201)	1:51:A:LYS:HE3	1:114:A:GLU:HB2	16	0.22
(2,3201)	1:51:A:LYS:HE3	1:114:A:GLU:HB2	17	0.22
(2,3085)	1:21:A:TYR:HD2	1:20:A:GLU:HB2	13	0.22
(2,2960)	1:52:A:LEU:HA	1:114:A:GLU:HG3	9	0.22
(2,2960)	1:52:A:LEU:HA	1:114:A:GLU:HG3	19	0.22
(2,2960)	1:52:A:LEU:HA	1:114:A:GLU:HG3	20	0.22
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	18	0.22
(2,2825)	1:25:A:LYS:HB3	1:26:A:ASP:HB2	17	0.22
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	3	0.22
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	19	0.22
(2,2806)	1:15:A:SER:HB2	1:38:A:ASN:HB2	7	0.22
(2,2806)	1:15:A:SER:HB3	1:38:A:ASN:HB2	12	0.22
(2,2806)	1:15:A:SER:HB2	1:38:A:ASN:HB2	15	0.22
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	8	0.22
(2,2704)	1:120:A:PHE:H	1:69:A:ILE:HB	10	0.22
(2,2658)	1:81:A:VAL:HG22	1:79:A:TYR:HB2	17	0.22
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	1	0.22
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	3	0.22
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	4	0.22
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	5	0.22
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	17	0.22
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	18	0.22
(2,2538)	1:115:A:TYR:HD1	1:118:A:LEU:HB3	12	0.22
(2,2372)	1:34:A:ILE:HG22	1:21:A:TYR:HA	12	0.22
(2,2364)	1:93:A:ILE:HG21	1:90:A:ALA:HA	2	0.22
(2,2179)	1:108:A:VAL:HG11	1:105:A:ASN:HA	7	0.22
(2,2174)	1:99:A:ILE:HD12	1:89:A:LYS:HA	1	0.22
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	19	0.22
(2,2081)	1:43:A:GLU:HG3	1:41:A:TYR:HA	20	0.22
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	14	0.22
(2,1892)	1:8:A:ILE:HG23	1:8:A:ILE:HA	18	0.22
(2,1891)	1:63:A:LEU:HD23	1:62:A:SER:HB3	1	0.22
(2,1891)	1:63:A:LEU:HD23	1:62:A:SER:HB3	19	0.22
(2,1877)	1:137:A:GLU:HB2	1:136:A:SER:HB2	8	0.22
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	9	0.22
(2,1847)	1:78:A:GLU:HB3	1:73:A:SER:HB2	11	0.22
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB2	7	0.22
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB3	12	0.22
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB2	15	0.22
(2,1808)	1:92:A:SER:HB3	1:91:A:ILE:HA	12	0.22
(2,1718)	1:64:A:VAL:HB	1:24:A:ILE:HA	15	0.22
(2,1660)	1:130:A:THR:HG22	1:132:A:GLU:H	10	0.22
(2,1542)	1:31:A:LYS:HG2	1:30:A:GLY:H	8	0.22
(2,1541)	1:32:A:LEU:HB3	1:30:A:GLY:H	10	0.22
(2,1541)	1:22:A:VAL:HB	1:30:A:GLY:H	12	0.22
(2,1540)	1:31:A:LYS:HB3	1:30:A:GLY:H	15	0.22
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	2	0.22
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	14	0.22
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	17	0.22
(2,1447)	1:22:A:VAL:HG21	1:23:A:THR:H	1	0.22
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	6	0.22
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	13	0.22
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	18	0.22
(2,1401)	1:106:A:VAL:HG12	1:105:A:ASN:HD22	8	0.22
(2,1388)	1:22:A:VAL:HG11	1:21:A:TYR:H	15	0.22
(2,1255)	1:28:A:LEU:HD23	1:54:A:SER:H	2	0.22
(2,1248)	1:94:A:LEU:HD11	1:95:A:LEU:H	15	0.22
(2,1236)	1:19:A:ALA:HB2	1:38:A:ASN:H	16	0.22
(2,1199)	1:102:A:VAL:HB	1:101:A:ASN:H	1	0.22
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	1	0.22
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	19	0.22
(2,1082)	1:24:A:ILE:HG22	1:25:A:LYS:H	7	0.22
(2,1082)	1:24:A:ILE:HG22	1:25:A:LYS:H	10	0.22
(2,1063)	1:23:A:THR:HG23	1:25:A:LYS:H	4	0.22
(2,1036)	1:43:A:GLU:HG2	1:33:A:LYS:H	16	0.22
(2,1027)	1:90:A:ALA:HB3	1:92:A:SER:H	11	0.22
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	18	0.22
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	4	0.22
(2,882)	1:28:A:LEU:HD21	1:28:A:LEU:H	12	0.22
(2,882)	1:28:A:LEU:HD21	1:28:A:LEU:H	18	0.22
(2,874)	1:49:A:VAL:HG23	1:48:A:GLU:H	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,863)	1:10:A:LEU:HD12	1:13:A:ILE:H	16	0.22
(2,862)	1:111:A:LEU:HD23	1:111:A:LEU:H	19	0.22
(2,850)	1:139:A:LEU:HD11	1:140:A:GLU:H	18	0.22
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	15	0.22
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	12	0.22
(2,819)	1:112:A:LEU:HB2	1:111:A:LEU:H	3	0.22
(2,764)	1:29:A:ASP:HB3	1:28:A:LEU:H	3	0.22
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	6	0.22
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	19	0.22
(2,598)	1:24:A:ILE:HG22	1:52:A:LEU:H	18	0.22
(2,597)	1:52:A:LEU:HD12	1:52:A:LEU:H	8	0.22
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	20	0.22
(2,571)	1:118:A:LEU:HD13	1:52:A:LEU:H	19	0.22
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	5	0.22
(2,544)	1:10:A:LEU:HG	1:10:A:LEU:H	11	0.22
(2,544)	1:10:A:LEU:HG	1:10:A:LEU:H	12	0.22
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	17	0.22
(2,209)	1:40:A:PHE:HB2	1:36:A:LEU:H	4	0.22
(2,161)	1:69:A:ILE:HG21	1:70:A:PHE:H	15	0.22
(2,158)	1:122:A:ILE:HG21	1:123:A:LEU:H	16	0.22
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	7	0.22
(2,108)	1:67:A:PRO:HA	1:120:A:PHE:H	14	0.22
(2,95)	1:70:A:PHE:HD1	1:122:A:ILE:H	11	0.22
(2,80)	1:34:A:ILE:HG23	1:35:A:ARG:H	20	0.22
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE2	7	0.21
(2,4659)	1:21:A:TYR:HB3	1:21:A:TYR:HE1	18	0.21
(2,4644)	1:123:A:LEU:HA	1:79:A:TYR:HE1	4	0.21
(2,4644)	1:123:A:LEU:HA	1:79:A:TYR:HE2	7	0.21
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	11	0.21
(2,4474)	1:36:A:LEU:HD21	1:41:A:TYR:HD2	12	0.21
(2,4398)	1:113:A:ARG:HA	1:113:A:ARG:HD2	7	0.21
(2,4320)	1:24:A:ILE:HB	1:66:A:ILE:HG22	5	0.21
(2,4320)	1:24:A:ILE:HB	1:66:A:ILE:HG23	8	0.21
(2,4225)	1:23:A:THR:HG22	1:62:A:SER:HB2	12	0.21
(2,4222)	1:72:A:LYS:HB3	1:73:A:SER:HB2	19	0.21
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD13	5	0.21
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD12	1	0.21
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD11	14	0.21
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD11	3	0.21
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD11	5	0.21
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD12	18	0.21
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	4	0.21
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	4	0.21
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	5	0.21
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	5	0.21
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	5	0.21
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG23	1	0.21
(2,4095)	1:49:A:VAL:H	1:66:A:ILE:HD11	15	0.21
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD13	17	0.21
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	4	0.21
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG22	15	0.21
(2,4020)	1:118:A:LEU:HB3	1:44:A:ILE:HG22	5	0.21
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG22	4	0.21
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG23	7	0.21
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG22	15	0.21
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG21	19	0.21
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG22	4	0.21
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG21	2	0.21
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG22	11	0.21
(2,3911)	1:70:A:PHE:HE1	1:103:A:ILE:HG23	19	0.21
(2,3905)	1:80:A:PHE:HE2	1:102:A:VAL:HG23	10	0.21
(2,3755)	1:135:A:LEU:HA	1:135:A:LEU:HD23	17	0.21
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG11	5	0.21
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG12	17	0.21
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG12	19	0.21
(2,3632)	1:94:A:LEU:HD12	1:95:A:LEU:HG	16	0.21
(2,3632)	1:94:A:LEU:HD13	1:95:A:LEU:HG	17	0.21
(2,3471)	1:118:A:LEU:HA	1:44:A:ILE:HG12	2	0.21
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	9	0.21
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	11	0.21
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD13	14	0.21
(2,3389)	1:41:A:TYR:HD2	1:36:A:LEU:HG	12	0.21
(2,3347)	1:120:A:PHE:HD2	1:69:A:ILE:HG12	2	0.21
(2,3344)	1:14:A:PHE:HE2	1:71:A:ILE:HG13	13	0.21
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD12	3	0.21
(2,3265)	1:94:A:LEU:HD12	1:91:A:ILE:HG12	8	0.21
(2,3085)	1:21:A:TYR:HD2	1:20:A:GLU:HB2	7	0.21
(2,3050)	1:142:A:HIS:HD2	1:142:A:HIS:HB3	20	0.21
(2,2955)	1:75:A:GLU:HA	1:75:A:GLU:HG2	16	0.21
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	7	0.21
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	10	0.21
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	11	0.21
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2658)	1:81:A:VAL:HG21	1:79:A:TYR:HB2	3	0.21
(2,2658)	1:81:A:VAL:HG22	1:79:A:TYR:HB2	6	0.21
(2,2653)	1:95:A:LEU:HD12	1:107:A:ASP:HB2	3	0.21
(2,2542)	1:115:A:TYR:HD2	1:111:A:LEU:HB2	2	0.21
(2,2538)	1:115:A:TYR:HD2	1:118:A:LEU:HB3	14	0.21
(2,2494)	1:10:A:LEU:HB2	1:9:A:GLY:HA2	3	0.21
(2,2490)	1:31:A:LYS:HG2	1:30:A:GLY:HA3	7	0.21
(2,2490)	1:31:A:LYS:HG2	1:30:A:GLY:HA3	8	0.21
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	19	0.21
(2,2375)	1:104:A:LEU:HD21	1:78:A:GLU:HA	11	0.21
(2,2143)	1:133:A:THR:HG23	1:134:A:GLU:HA	10	0.21
(2,2099)	1:134:A:GLU:HG2	1:134:A:GLU:HA	12	0.21
(2,2099)	1:134:A:GLU:HG2	1:134:A:GLU:HA	15	0.21
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	1	0.21
(2,1990)	1:14:A:PHE:HD2	1:11:A:LYS:HA	3	0.21
(2,1948)	1:92:A:SER:H	1:99:A:ILE:HA	9	0.21
(2,1891)	1:63:A:LEU:HD22	1:62:A:SER:HB3	3	0.21
(2,1891)	1:63:A:LEU:HD22	1:62:A:SER:HB3	14	0.21
(2,1877)	1:135:A:LEU:HB2	1:136:A:SER:HB2	9	0.21
(2,1877)	1:135:A:LEU:HB3	1:136:A:SER:HB3	11	0.21
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	4	0.21
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	7	0.21
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	10	0.21
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	17	0.21
(2,1731)	1:56:A:ILE:HG23	1:24:A:ILE:HA	6	0.21
(2,1654)	1:41:A:TYR:HB3	1:36:A:LEU:H	11	0.21
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	9	0.21
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	17	0.21
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	6	0.21
(2,1599)	1:62:A:SER:HA	1:26:A:ASP:H	7	0.21
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	8	0.21
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	11	0.21
(2,1540)	1:31:A:LYS:HB3	1:30:A:GLY:H	9	0.21
(2,1499)	1:93:A:ILE:HG22	1:96:A:GLY:H	4	0.21
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	20	0.21
(2,1435)	1:31:A:LYS:HB3	1:23:A:THR:H	13	0.21
(2,1386)	1:65:A:LYS:HD3	1:21:A:TYR:H	11	0.21
(2,1350)	1:50:A:GLU:HB3	1:53:A:SER:H	8	0.21
(2,1255)	1:52:A:LEU:HD12	1:54:A:SER:H	12	0.21
(2,1248)	1:94:A:LEU:HD11	1:95:A:LEU:H	9	0.21
(2,1200)	1:36:A:LEU:HB3	1:41:A:TYR:H	5	0.21
(2,1199)	1:102:A:VAL:HB	1:101:A:ASN:H	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1180)	1:45:A:LYS:HE2	1:47:A:ASP:H	9	0.21
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	4	0.21
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	13	0.21
(2,1166)	1:124:A:SER:HB3	1:124:A:SER:H	17	0.21
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	20	0.21
(2,1104)	1:37:A:ASN:H	1:20:A:GLU:H	3	0.21
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	13	0.21
(2,1082)	1:24:A:ILE:HG22	1:25:A:LYS:H	8	0.21
(2,1082)	1:24:A:ILE:HG23	1:25:A:LYS:H	13	0.21
(2,1030)	1:22:A:VAL:HB	1:29:A:ASP:H	10	0.21
(2,1027)	1:90:A:ALA:HB2	1:92:A:SER:H	12	0.21
(2,1019)	1:67:A:PRO:HB3	1:66:A:ILE:H	17	0.21
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	8	0.21
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	3	0.21
(2,895)	1:91:A:ILE:HD13	1:88:A:LYS:H	7	0.21
(2,882)	1:28:A:LEU:HD21	1:28:A:LEU:H	5	0.21
(2,882)	1:28:A:LEU:HD23	1:28:A:LEU:H	14	0.21
(2,877)	1:60:A:LEU:HD21	1:86:A:TRP:H	13	0.21
(2,871)	1:119:A:ILE:HD12	1:119:A:ILE:H	16	0.21
(2,862)	1:95:A:LEU:HD21	1:111:A:LEU:H	7	0.21
(2,831)	1:119:A:ILE:HD11	1:112:A:LEU:H	9	0.21
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	4	0.21
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	2	0.21
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	8	0.21
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	7	0.21
(2,605)	1:28:A:LEU:HD23	1:51:A:LYS:H	2	0.21
(2,605)	1:28:A:LEU:HD21	1:51:A:LYS:H	6	0.21
(2,605)	1:28:A:LEU:HD22	1:51:A:LYS:H	8	0.21
(2,597)	1:52:A:LEU:HD12	1:52:A:LEU:H	3	0.21
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	14	0.21
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	16	0.21
(2,571)	1:118:A:LEU:HD12	1:52:A:LEU:H	4	0.21
(2,571)	1:118:A:LEU:HD13	1:52:A:LEU:H	5	0.21
(2,568)	1:49:A:VAL:HG11	1:50:A:GLU:H	9	0.21
(2,568)	1:49:A:VAL:HG12	1:50:A:GLU:H	9	0.21
(2,568)	1:49:A:VAL:HG13	1:50:A:GLU:H	9	0.21
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	3	0.21
(2,401)	1:70:A:PHE:HE2	1:69:A:ILE:H	18	0.21
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	5	0.21
(2,331)	1:33:A:LYS:HB2	1:32:A:LEU:H	16	0.21
(2,231)	1:34:A:ILE:HB	1:36:A:LEU:H	20	0.21
(2,225)	1:98:A:GLU:HG2	1:99:A:ILE:H	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	15	0.21
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	15	0.21
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	15	0.21
(2,158)	1:122:A:ILE:HG22	1:123:A:LEU:H	1	0.21
(2,158)	1:122:A:ILE:HG21	1:123:A:LEU:H	7	0.21
(2,154)	1:71:A:ILE:HD11	1:122:A:ILE:H	2	0.21
(2,154)	1:71:A:ILE:HD13	1:122:A:ILE:H	13	0.21
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	5	0.21
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	7	0.21
(2,138)	1:67:A:PRO:HB3	1:120:A:PHE:H	17	0.21
(2,95)	1:70:A:PHE:HD2	1:122:A:ILE:H	8	0.21
(2,80)	1:34:A:ILE:HG22	1:35:A:ARG:H	1	0.21
(2,80)	1:34:A:ILE:HG23	1:35:A:ARG:H	15	0.21
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	5	0.21
(2,34)	1:71:A:ILE:HG21	1:72:A:LYS:H	10	0.21
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	13	0.21
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE1	15	0.2
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE1	2	0.2
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE2	17	0.2
(2,4483)	1:122:A:ILE:HA	1:14:A:PHE:HE1	1	0.2
(2,4474)	1:36:A:LEU:HD22	1:41:A:TYR:HD1	11	0.2
(2,4465)	1:118:A:LEU:HD12	1:115:A:TYR:HD2	13	0.2
(2,4465)	1:118:A:LEU:HD12	1:115:A:TYR:HD2	14	0.2
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD1	11	0.2
(2,4459)	1:33:A:LYS:HB3	1:41:A:TYR:HD1	15	0.2
(2,4450)	1:132:A:GLU:HB2	1:129:A:TYR:HD1	11	0.2
(2,4398)	1:52:A:LEU:HA	1:55:A:ARG:HD3	6	0.2
(2,4377)	1:135:A:LEU:HD22	1:134:A:GLU:HG3	5	0.2
(2,4377)	1:135:A:LEU:HD21	1:134:A:GLU:HG3	10	0.2
(2,4333)	1:18:A:PRO:HD3	1:122:A:ILE:HD12	13	0.2
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB2	19	0.2
(2,4276)	1:111:A:LEU:HD23	1:114:A:GLU:HB2	15	0.2
(2,4225)	1:23:A:THR:HG22	1:62:A:SER:HB2	2	0.2
(2,4225)	1:23:A:THR:HG23	1:62:A:SER:HB2	3	0.2
(2,4225)	1:23:A:THR:HG23	1:62:A:SER:HB2	8	0.2
(2,4225)	1:23:A:THR:HG22	1:62:A:SER:HB2	9	0.2
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD12	2	0.2
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD11	5	0.2
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD13	18	0.2
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD12	11	0.2
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	17	0.2
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	17	0.2
(2,4136)	1:76:A:ILE:HA	1:76:A:ILE:HD11	6	0.2
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD11	4	0.2
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD12	12	0.2
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD13	14	0.2
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	8	0.2
(2,4020)	1:49:A:VAL:HB	1:44:A:ILE:HG21	4	0.2
(2,4012)	1:68:A:PHE:HB3	1:66:A:ILE:HG21	8	0.2
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG22	2	0.2
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG23	3	0.2
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG23	7	0.2
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG21	15	0.2
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG22	15	0.2
(2,3928)	1:70:A:PHE:HZ	1:103:A:ILE:HG23	9	0.2
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB1	1	0.2
(2,3799)	1:107:A:ASP:HB3	1:95:A:LEU:HD23	6	0.2
(2,3720)	1:86:A:TRP:HH2	1:63:A:LEU:HD22	6	0.2
(2,3715)	1:54:A:SER:H	1:28:A:LEU:HD22	7	0.2
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG12	13	0.2
(2,3601)	1:56:A:ILE:HB	1:52:A:LEU:HD12	8	0.2
(2,3471)	1:32:A:LEU:HA	1:44:A:ILE:HG13	15	0.2
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	17	0.2
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG3	19	0.2
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	1	0.2
(2,3405)	1:115:A:TYR:HE1	1:118:A:LEU:HD12	7	0.2
(2,3304)	1:50:A:GLU:H	1:118:A:LEU:HD23	18	0.2
(2,3281)	1:72:A:LYS:H	1:71:A:ILE:HG13	13	0.2
(2,3265)	1:94:A:LEU:HD13	1:91:A:ILE:HG12	11	0.2
(2,2973)	1:109:A:GLU:HA	1:109:A:GLU:HG2	9	0.2
(2,2954)	1:132:A:GLU:HA	1:132:A:GLU:HG2	3	0.2
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	2	0.2
(2,2822)	1:118:A:LEU:HB3	1:115:A:TYR:HB2	5	0.2
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	15	0.2
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	17	0.2
(2,2538)	1:115:A:TYR:HD1	1:118:A:LEU:HB3	10	0.2
(2,2496)	1:46:A:LYS:HG3	1:30:A:GLY:HA2	8	0.2
(2,2496)	1:46:A:LYS:HG3	1:30:A:GLY:HA2	20	0.2
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	20	0.2
(2,2473)	1:122:A:ILE:HD12	1:18:A:PRO:HD3	13	0.2
(2,2179)	1:108:A:VAL:HG13	1:105:A:ASN:HA	5	0.2
(2,2175)	1:94:A:LEU:HD23	1:52:A:LEU:HA	17	0.2
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1894)	1:76:A:ILE:HD11	1:76:A:ILE:HA	6	0.2
(2,1781)	1:68:A:PHE:HE2	1:91:A:ILE:HA	7	0.2
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	5	0.2
(2,1632)	1:138:A:MET:HB3	1:136:A:SER:H	10	0.2
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	7	0.2
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	15	0.2
(2,1601)	1:20:A:GLU:HG3	1:34:A:ILE:H	16	0.2
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	1	0.2
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	16	0.2
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	19	0.2
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	3	0.2
(2,1541)	1:22:A:VAL:HB	1:30:A:GLY:H	18	0.2
(2,1520)	1:25:A:LYS:HB3	1:62:A:SER:H	6	0.2
(2,1499)	1:93:A:ILE:HG21	1:96:A:GLY:H	15	0.2
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	11	0.2
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	15	0.2
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	16	0.2
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	19	0.2
(2,1486)	1:71:A:ILE:HG13	1:83:A:GLY:H	13	0.2
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	19	0.2
(2,1447)	1:22:A:VAL:HG22	1:23:A:THR:H	7	0.2
(2,1447)	1:22:A:VAL:HG21	1:23:A:THR:H	17	0.2
(2,1445)	1:65:A:LYS:HG2	1:23:A:THR:H	8	0.2
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	2	0.2
(2,1389)	1:106:A:VAL:HG11	1:105:A:ASN:HD21	1	0.2
(2,1386)	1:65:A:LYS:HD2	1:21:A:TYR:H	20	0.2
(2,1350)	1:50:A:GLU:HB3	1:53:A:SER:H	4	0.2
(2,1255)	1:52:A:LEU:HD11	1:54:A:SER:H	4	0.2
(2,1248)	1:94:A:LEU:HD12	1:95:A:LEU:H	18	0.2
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	10	0.2
(2,1236)	1:36:A:LEU:HD12	1:38:A:ASN:H	20	0.2
(2,1228)	1:123:A:LEU:HD22	1:124:A:SER:H	19	0.2
(2,1222)	1:33:A:LYS:HD3	1:41:A:TYR:H	19	0.2
(2,1219)	1:65:A:LYS:HD2	1:22:A:VAL:H	16	0.2
(2,1199)	1:99:A:ILE:HB	1:101:A:ASN:H	10	0.2
(2,1191)	1:131:A:GLU:HG2	1:133:A:THR:H	4	0.2
(2,1188)	1:37:A:ASN:HB2	1:15:A:SER:H	5	0.2
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	6	0.2
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	14	0.2
(2,1082)	1:24:A:ILE:HG22	1:25:A:LYS:H	2	0.2
(2,980)	1:141:A:HIS:HB2	1:141:A:HIS:H	19	0.2
(2,962)	1:95:A:LEU:HA	1:97:A:ARG:H	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	6	0.2
(2,895)	1:91:A:ILE:HD12	1:88:A:LYS:H	8	0.2
(2,886)	1:24:A:ILE:HG22	1:26:A:ASP:H	8	0.2
(2,871)	1:119:A:ILE:HD13	1:119:A:ILE:H	4	0.2
(2,862)	1:111:A:LEU:HD21	1:111:A:LEU:H	8	0.2
(2,862)	1:111:A:LEU:HD23	1:111:A:LEU:H	16	0.2
(2,862)	1:95:A:LEU:HD22	1:111:A:LEU:H	18	0.2
(2,850)	1:139:A:LEU:HD12	1:140:A:GLU:H	8	0.2
(2,848)	1:27:A:ALA:HB2	1:26:A:ASP:H	9	0.2
(2,848)	1:27:A:ALA:HB2	1:26:A:ASP:H	11	0.2
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	5	0.2
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	10	0.2
(2,819)	1:112:A:LEU:HB2	1:111:A:LEU:H	4	0.2
(2,791)	1:111:A:LEU:HB3	1:112:A:LEU:H	17	0.2
(2,764)	1:29:A:ASP:HB3	1:28:A:LEU:H	7	0.2
(2,760)	1:33:A:LYS:HE2	1:34:A:ILE:H	19	0.2
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	20	0.2
(2,663)	1:115:A:TYR:HD2	1:112:A:LEU:H	18	0.2
(2,582)	1:56:A:ILE:HG13	1:55:A:ARG:H	12	0.2
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	20	0.2
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	2	0.2
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	13	0.2
(2,348)	1:58:A:LEU:HD21	1:61:A:TRP:H	3	0.2
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	20	0.2
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	14	0.2
(2,245)	1:44:A:ILE:HD13	1:44:A:ILE:H	4	0.2
(2,185)	1:35:A:ARG:HE	1:36:A:LEU:H	10	0.2
(2,160)	1:121:A:ILE:HG21	1:70:A:PHE:H	11	0.2
(2,154)	1:71:A:ILE:HD11	1:122:A:ILE:H	19	0.2
(2,154)	1:71:A:ILE:HD12	1:122:A:ILE:H	20	0.2
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	20	0.2
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	5	0.2
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	14	0.2
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE1	11	0.19
(2,4667)	1:94:A:LEU:HD22	1:115:A:TYR:HE1	1	0.19
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE1	6	0.19
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE2	4	0.19
(2,4648)	1:20:A:GLU:HA	1:21:A:TYR:HE1	11	0.19
(2,4519)	1:119:A:ILE:HG22	1:68:A:PHE:HD1	9	0.19
(2,4512)	1:121:A:ILE:HD12	1:79:A:TYR:HD2	12	0.19
(2,4505)	1:122:A:ILE:HD12	1:14:A:PHE:HD2	8	0.19
(2,4474)	1:36:A:LEU:HD23	1:41:A:TYR:HD1	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4468)	1:35:A:ARG:HB2	1:41:A:TYR:HD2	7	0.19
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD2	13	0.19
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	1	0.19
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	8	0.19
(2,4398)	1:52:A:LEU:HA	1:55:A:ARG:HD2	2	0.19
(2,4398)	1:52:A:LEU:HA	1:55:A:ARG:HD3	20	0.19
(2,4377)	1:135:A:LEU:HD23	1:134:A:GLU:HG3	17	0.19
(2,4318)	1:46:A:LYS:HB2	1:27:A:ALA:HB1	4	0.19
(2,4288)	1:115:A:TYR:HB2	1:52:A:LEU:HD11	20	0.19
(2,4254)	1:45:A:LYS:HG2	1:47:A:ASP:HB3	3	0.19
(2,4225)	1:23:A:THR:HG21	1:62:A:SER:HB2	11	0.19
(2,4225)	1:23:A:THR:HG21	1:62:A:SER:HB2	18	0.19
(2,4207)	1:70:A:PHE:HE2	1:91:A:ILE:HD11	14	0.19
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD13	13	0.19
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD11	20	0.19
(2,4092)	1:14:A:PHE:HD2	1:122:A:ILE:HD12	8	0.19
(2,4080)	1:28:A:LEU:H	1:24:A:ILE:HG22	2	0.19
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG21	9	0.19
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG21	7	0.19
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG21	16	0.19
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG21	10	0.19
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG23	17	0.19
(2,3911)	1:70:A:PHE:HE1	1:103:A:ILE:HG22	12	0.19
(2,3911)	1:70:A:PHE:HE2	1:103:A:ILE:HG22	16	0.19
(2,3911)	1:70:A:PHE:HE1	1:103:A:ILE:HG23	18	0.19
(2,3908)	1:48:A:GLU:H	1:44:A:ILE:HG21	19	0.19
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG22	8	0.19
(2,3632)	1:94:A:LEU:HD13	1:95:A:LEU:HG	14	0.19
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	2	0.19
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	7	0.19
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	10	0.19
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	18	0.19
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD11	17	0.19
(2,3435)	1:23:A:THR:HB	1:65:A:LYS:HG3	2	0.19
(2,3281)	1:72:A:LYS:H	1:71:A:ILE:HG13	7	0.19
(2,3265)	1:94:A:LEU:HD12	1:91:A:ILE:HG12	13	0.19
(2,3108)	1:42:A:HIS:HA	1:43:A:GLU:HB2	5	0.19
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	9	0.19
(2,3075)	1:86:A:TRP:HD1	1:65:A:LYS:HD2	11	0.19
(2,3065)	1:70:A:PHE:HD2	1:81:A:VAL:HB	11	0.19
(2,3065)	1:70:A:PHE:HD1	1:81:A:VAL:HB	12	0.19
(2,3016)	1:24:A:ILE:HG23	1:25:A:LYS:HB2	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	15	0.19
(2,2954)	1:137:A:GLU:HA	1:137:A:GLU:HG2	8	0.19
(2,2953)	1:134:A:GLU:HA	1:134:A:GLU:HG3	4	0.19
(2,2827)	1:50:A:GLU:HB2	1:47:A:ASP:HB3	12	0.19
(2,2825)	1:31:A:LYS:HB3	1:26:A:ASP:HB2	18	0.19
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	13	0.19
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	9	0.19
(2,2542)	1:115:A:TYR:HD1	1:111:A:LEU:HB2	12	0.19
(2,2538)	1:115:A:TYR:HD1	1:118:A:LEU:HB3	4	0.19
(2,2496)	1:32:A:LEU:HB2	1:30:A:GLY:HA2	18	0.19
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	13	0.19
(2,2340)	1:114:A:GLU:HB3	1:115:A:TYR:HA	13	0.19
(2,2318)	1:110:A:LYS:HB2	1:107:A:ASP:HA	9	0.19
(2,2235)	1:95:A:LEU:H	1:90:A:ALA:HA	12	0.19
(2,2179)	1:108:A:VAL:HG12	1:105:A:ASN:HA	3	0.19
(2,2145)	1:46:A:LYS:HD2	1:46:A:LYS:HA	13	0.19
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	13	0.19
(2,2099)	1:131:A:GLU:HG2	1:131:A:GLU:HA	2	0.19
(2,2099)	1:134:A:GLU:HG2	1:134:A:GLU:HA	10	0.19
(2,2084)	1:31:A:LYS:HB3	1:22:A:VAL:HA	17	0.19
(2,1948)	1:92:A:SER:H	1:99:A:ILE:HA	7	0.19
(2,1891)	1:63:A:LEU:HD22	1:62:A:SER:HB3	12	0.19
(2,1866)	1:139:A:LEU:HB2	1:136:A:SER:HB3	4	0.19
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	16	0.19
(2,1781)	1:68:A:PHE:HE1	1:91:A:ILE:HA	14	0.19
(2,1717)	1:49:A:VAL:HB	1:24:A:ILE:HA	6	0.19
(2,1660)	1:130:A:THR:HG21	1:132:A:GLU:H	15	0.19
(2,1654)	1:41:A:TYR:HB3	1:36:A:LEU:H	2	0.19
(2,1654)	1:41:A:TYR:HB3	1:36:A:LEU:H	10	0.19
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	16	0.19
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	3	0.19
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	16	0.19
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	17	0.19
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	20	0.19
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	7	0.19
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	15	0.19
(2,1557)	1:24:A:ILE:HD12	1:61:A:TRP:HE1	19	0.19
(2,1540)	1:46:A:LYS:HB2	1:30:A:GLY:H	1	0.19
(2,1540)	1:31:A:LYS:HB3	1:30:A:GLY:H	11	0.19
(2,1499)	1:93:A:ILE:HG22	1:96:A:GLY:H	18	0.19
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	1	0.19
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	3	0.19
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	7	0.19
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	16	0.19
(2,1447)	1:22:A:VAL:HG22	1:23:A:THR:H	16	0.19
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	1	0.19
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	7	0.19
(2,1350)	1:50:A:GLU:HB3	1:53:A:SER:H	3	0.19
(2,1350)	1:51:A:LYS:HB2	1:53:A:SER:H	6	0.19
(2,1228)	1:122:A:ILE:HG21	1:124:A:SER:H	9	0.19
(2,1222)	1:33:A:LYS:HD3	1:41:A:TYR:H	13	0.19
(2,1219)	1:65:A:LYS:HD2	1:22:A:VAL:H	7	0.19
(2,1179)	1:35:A:ARG:HD3	1:20:A:GLU:H	2	0.19
(2,1179)	1:35:A:ARG:HD3	1:20:A:GLU:H	10	0.19
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	11	0.19
(2,1179)	1:35:A:ARG:HD3	1:20:A:GLU:H	17	0.19
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	1	0.19
(2,1082)	1:24:A:ILE:HG23	1:25:A:LYS:H	16	0.19
(2,1063)	1:23:A:THR:HG22	1:25:A:LYS:H	2	0.19
(2,1027)	1:90:A:ALA:HB2	1:92:A:SER:H	19	0.19
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	13	0.19
(2,882)	1:28:A:LEU:HD21	1:28:A:LEU:H	15	0.19
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	10	0.19
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	20	0.19
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	4	0.19
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	11	0.19
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	18	0.19
(2,815)	1:85:A:GLN:HG3	1:87:A:ASN:H	15	0.19
(2,747)	1:109:A:GLU:HA	1:111:A:LEU:H	13	0.19
(2,583)	1:94:A:LEU:HD23	1:55:A:ARG:H	13	0.19
(2,582)	1:56:A:ILE:HG13	1:55:A:ARG:H	13	0.19
(2,576)	1:133:A:THR:HG22	1:137:A:GLU:H	12	0.19
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	12	0.19
(2,571)	1:118:A:LEU:HD13	1:52:A:LEU:H	14	0.19
(2,571)	1:118:A:LEU:HD11	1:52:A:LEU:H	20	0.19
(2,401)	1:70:A:PHE:HE2	1:69:A:ILE:H	1	0.19
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	6	0.19
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	7	0.19
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	14	0.19
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	5	0.19
(2,253)	1:22:A:VAL:HG21	1:27:A:ALA:H	14	0.19
(2,185)	1:20:A:GLU:H	1:36:A:LEU:H	1	0.19
(2,166)	1:22:A:VAL:HG11	1:31:A:LYS:H	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:22:A:VAL:HG12	1:31:A:LYS:H	18	0.19
(2,166)	1:22:A:VAL:HG13	1:31:A:LYS:H	18	0.19
(2,156)	1:69:A:ILE:HD11	1:120:A:PHE:H	2	0.19
(2,156)	1:69:A:ILE:HD11	1:120:A:PHE:H	7	0.19
(2,154)	1:71:A:ILE:HD13	1:122:A:ILE:H	1	0.19
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	8	0.19
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	2	0.19
(2,95)	1:70:A:PHE:HD2	1:122:A:ILE:H	18	0.19
(2,84)	1:24:A:ILE:HG21	1:61:A:TRP:HE1	18	0.19
(2,80)	1:34:A:ILE:HG21	1:35:A:ARG:H	13	0.19
(2,80)	1:34:A:ILE:HG22	1:35:A:ARG:H	14	0.19
(2,80)	1:34:A:ILE:HG23	1:35:A:ARG:H	17	0.19
(2,80)	1:34:A:ILE:HG22	1:35:A:ARG:H	18	0.19
(2,34)	1:71:A:ILE:HG22	1:72:A:LYS:H	3	0.19
(2,33)	1:46:A:LYS:HD3	1:46:A:LYS:H	3	0.19
(2,33)	1:46:A:LYS:HD3	1:46:A:LYS:H	4	0.19
(2,4699)	1:60:A:LEU:H	1:59:A:TYR:HE1	19	0.18
(2,4689)	1:123:A:LEU:HD21	1:79:A:TYR:HD2	13	0.18
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE1	3	0.18
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE2	5	0.18
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE1	6	0.18
(2,4659)	1:21:A:TYR:HB3	1:21:A:TYR:HE1	10	0.18
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE1	15	0.18
(2,4474)	1:36:A:LEU:HD22	1:41:A:TYR:HD1	3	0.18
(2,4474)	1:36:A:LEU:HD21	1:41:A:TYR:HD2	9	0.18
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD2	12	0.18
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	12	0.18
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	16	0.18
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD13	19	0.18
(2,4324)	1:91:A:ILE:H	1:56:A:ILE:HD11	8	0.18
(2,4291)	1:52:A:LEU:HG	1:94:A:LEU:HD13	6	0.18
(2,4225)	1:23:A:THR:HG23	1:62:A:SER:HB2	4	0.18
(2,4207)	1:70:A:PHE:HE1	1:91:A:ILE:HD11	6	0.18
(2,4207)	1:70:A:PHE:HE2	1:91:A:ILE:HD11	11	0.18
(2,4207)	1:68:A:PHE:HE2	1:91:A:ILE:HD13	16	0.18
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD12	12	0.18
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD12	2	0.18
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD13	8	0.18
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD11	20	0.18
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD13	19	0.18
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG21	16	0.18
(2,4020)	1:118:A:LEU:HB3	1:44:A:ILE:HG22	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG22	1	0.18
(2,3966)	1:89:A:LYS:HA	1:99:A:ILE:HG23	18	0.18
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG23	4	0.18
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG21	14	0.18
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG23	10	0.18
(2,3911)	1:70:A:PHE:HE2	1:103:A:ILE:HG23	15	0.18
(2,3905)	1:80:A:PHE:HE1	1:102:A:VAL:HG23	16	0.18
(2,3826)	1:79:A:TYR:HB2	1:108:A:VAL:HG13	2	0.18
(2,3632)	1:94:A:LEU:HD13	1:95:A:LEU:HG	1	0.18
(2,3632)	1:94:A:LEU:HD11	1:95:A:LEU:HG	9	0.18
(2,3606)	1:56:A:ILE:HG13	1:57:A:PRO:HG3	11	0.18
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG23	14	0.18
(2,3471)	1:118:A:LEU:HA	1:44:A:ILE:HG12	1	0.18
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	10	0.18
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	18	0.18
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	4	0.18
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	12	0.18
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD12	9	0.18
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD12	9	0.18
(2,3331)	1:52:A:LEU:H	1:52:A:LEU:HD11	19	0.18
(2,3281)	1:72:A:LYS:H	1:71:A:ILE:HG13	11	0.18
(2,3265)	1:94:A:LEU:HD11	1:91:A:ILE:HG12	9	0.18
(2,3108)	1:42:A:HIS:HA	1:43:A:GLU:HB2	16	0.18
(2,3085)	1:21:A:TYR:HD2	1:20:A:GLU:HB2	5	0.18
(2,3085)	1:21:A:TYR:HD1	1:20:A:GLU:HB2	12	0.18
(2,3065)	1:70:A:PHE:HD2	1:81:A:VAL:HB	10	0.18
(2,3065)	1:70:A:PHE:HD2	1:81:A:VAL:HB	15	0.18
(2,3065)	1:70:A:PHE:HD1	1:81:A:VAL:HB	18	0.18
(2,2960)	1:52:A:LEU:HA	1:114:A:GLU:HG3	17	0.18
(2,2954)	1:137:A:GLU:HA	1:137:A:GLU:HG2	9	0.18
(2,2841)	1:72:A:LYS:HG2	1:105:A:ASN:HB3	9	0.18
(2,2825)	1:31:A:LYS:HB3	1:26:A:ASP:HB2	6	0.18
(2,2822)	1:118:A:LEU:HB3	1:115:A:TYR:HB2	9	0.18
(2,2819)	1:81:A:VAL:HB	1:101:A:ASN:HB2	6	0.18
(2,2806)	1:15:A:SER:HB3	1:38:A:ASN:HB2	19	0.18
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	9	0.18
(2,2538)	1:115:A:TYR:HD2	1:118:A:LEU:HB3	9	0.18
(2,2490)	1:31:A:LYS:HG2	1:30:A:GLY:HA3	11	0.18
(2,2490)	1:31:A:LYS:HG2	1:30:A:GLY:HA3	18	0.18
(2,2473)	1:69:A:ILE:HD13	1:18:A:PRO:HD3	19	0.18
(2,2375)	1:104:A:LEU:HD23	1:78:A:GLU:HA	10	0.18
(2,2340)	1:114:A:GLU:HB3	1:115:A:TYR:HA	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2175)	1:94:A:LEU:HD22	1:52:A:LEU:HA	10	0.18
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	1	0.18
(2,2099)	1:131:A:GLU:HG2	1:131:A:GLU:HA	7	0.18
(2,2099)	1:134:A:GLU:HG2	1:134:A:GLU:HA	19	0.18
(2,1998)	1:115:A:TYR:HD1	1:112:A:LEU:HA	8	0.18
(2,1948)	1:92:A:SER:H	1:99:A:ILE:HA	18	0.18
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	1	0.18
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	14	0.18
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	17	0.18
(2,1899)	1:76:A:ILE:HD12	1:73:A:SER:HB3	17	0.18
(2,1891)	1:63:A:LEU:HD22	1:62:A:SER:HB3	4	0.18
(2,1891)	1:63:A:LEU:HD22	1:62:A:SER:HB3	9	0.18
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	12	0.18
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	18	0.18
(2,1833)	1:51:A:LYS:HB2	1:54:A:SER:HB2	10	0.18
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB3	19	0.18
(2,1787)	1:120:A:PHE:HE2	1:17:A:SER:HB3	9	0.18
(2,1781)	1:68:A:PHE:HE1	1:91:A:ILE:HA	19	0.18
(2,1773)	1:14:A:PHE:HE1	1:82:A:SER:HB3	1	0.18
(2,1731)	1:56:A:ILE:HG21	1:24:A:ILE:HA	12	0.18
(2,1731)	1:56:A:ILE:HG22	1:24:A:ILE:HA	15	0.18
(2,1718)	1:64:A:VAL:HB	1:24:A:ILE:HA	13	0.18
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	2	0.18
(2,1626)	1:139:A:LEU:HD11	1:136:A:SER:H	2	0.18
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	2	0.18
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	9	0.18
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	10	0.18
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	5	0.18
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	10	0.18
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	17	0.18
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	14	0.18
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	18	0.18
(2,1445)	1:65:A:LYS:HG2	1:23:A:THR:H	9	0.18
(2,1440)	1:20:A:GLU:HG2	1:35:A:ARG:HE	11	0.18
(2,1435)	1:31:A:LYS:HB3	1:23:A:THR:H	15	0.18
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	4	0.18
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	20	0.18
(2,1394)	1:64:A:VAL:HG22	1:87:A:ASN:HD22	11	0.18
(2,1388)	1:34:A:ILE:HG21	1:21:A:TYR:H	3	0.18
(2,1386)	1:65:A:LYS:HD2	1:21:A:TYR:H	6	0.18
(2,1367)	1:119:A:ILE:HB	1:116:A:THR:H	13	0.18
(2,1367)	1:45:A:LYS:HB2	1:116:A:THR:H	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	17	0.18
(2,1244)	1:34:A:ILE:HD11	1:20:A:GLU:H	2	0.18
(2,1191)	1:132:A:GLU:HG2	1:133:A:THR:H	16	0.18
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	3	0.18
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	15	0.18
(2,1104)	1:37:A:ASN:H	1:20:A:GLU:H	4	0.18
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	14	0.18
(2,1082)	1:24:A:ILE:HG22	1:25:A:LYS:H	5	0.18
(2,1082)	1:24:A:ILE:HG23	1:25:A:LYS:H	15	0.18
(2,1053)	1:112:A:LEU:HD13	1:109:A:GLU:H	9	0.18
(2,1036)	1:43:A:GLU:HG2	1:33:A:LYS:H	2	0.18
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	1	0.18
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	14	0.18
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	20	0.18
(2,877)	1:60:A:LEU:HD22	1:86:A:TRP:H	7	0.18
(2,871)	1:119:A:ILE:HD13	1:119:A:ILE:H	14	0.18
(2,862)	1:95:A:LEU:HD21	1:111:A:LEU:H	2	0.18
(2,862)	1:111:A:LEU:HD21	1:111:A:LEU:H	4	0.18
(2,848)	1:27:A:ALA:HB1	1:26:A:ASP:H	6	0.18
(2,831)	1:119:A:ILE:HD13	1:112:A:LEU:H	18	0.18
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	6	0.18
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	15	0.18
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	17	0.18
(2,784)	1:61:A:TRP:HB2	1:24:A:ILE:H	16	0.18
(2,677)	1:78:A:GLU:HA	1:103:A:ILE:H	5	0.18
(2,597)	1:52:A:LEU:HD12	1:52:A:LEU:H	9	0.18
(2,597)	1:52:A:LEU:HD11	1:52:A:LEU:H	19	0.18
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	8	0.18
(2,571)	1:118:A:LEU:HD12	1:52:A:LEU:H	8	0.18
(2,568)	1:49:A:VAL:HG11	1:50:A:GLU:H	2	0.18
(2,568)	1:49:A:VAL:HG12	1:50:A:GLU:H	2	0.18
(2,568)	1:49:A:VAL:HG13	1:50:A:GLU:H	2	0.18
(2,527)	1:72:A:LYS:HB2	1:79:A:TYR:H	16	0.18
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	7	0.18
(2,492)	1:105:A:ASN:HB3	1:79:A:TYR:H	11	0.18
(2,492)	1:105:A:ASN:HB2	1:79:A:TYR:H	14	0.18
(2,348)	1:58:A:LEU:HD22	1:61:A:TRP:H	4	0.18
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	1	0.18
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	3	0.18
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	10	0.18
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	18	0.18
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:22:A:VAL:HG21	1:31:A:LYS:H	6	0.18
(2,166)	1:22:A:VAL:HG22	1:31:A:LYS:H	6	0.18
(2,166)	1:22:A:VAL:HG23	1:31:A:LYS:H	6	0.18
(2,160)	1:121:A:ILE:HG22	1:70:A:PHE:H	4	0.18
(2,158)	1:122:A:ILE:HG23	1:123:A:LEU:H	18	0.18
(2,154)	1:71:A:ILE:HD11	1:122:A:ILE:H	12	0.18
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	8	0.18
(2,84)	1:24:A:ILE:HG23	1:61:A:TRP:HE1	8	0.18
(2,80)	1:34:A:ILE:HG22	1:35:A:ARG:H	2	0.18
(2,80)	1:34:A:ILE:HG23	1:35:A:ARG:H	9	0.18
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	11	0.18
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE1	3	0.17
(2,4659)	1:21:A:TYR:HB3	1:21:A:TYR:HE2	8	0.17
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE2	12	0.17
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE1	20	0.17
(2,4465)	1:118:A:LEU:HD12	1:115:A:TYR:HD2	9	0.17
(2,4291)	1:52:A:LEU:HG	1:94:A:LEU:HD11	4	0.17
(2,4236)	1:118:A:LEU:HD21	1:117:A:SER:HA	6	0.17
(2,4225)	1:23:A:THR:HG22	1:62:A:SER:HB2	5	0.17
(2,4207)	1:68:A:PHE:HE1	1:91:A:ILE:HD11	18	0.17
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD13	2	0.17
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD13	11	0.17
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	15	0.17
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	15	0.17
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	15	0.17
(2,4116)	1:115:A:TYR:HA	1:119:A:ILE:HD12	6	0.17
(2,4116)	1:115:A:TYR:HA	1:119:A:ILE:HD13	18	0.17
(2,4072)	1:90:A:ALA:H	1:93:A:ILE:HD13	8	0.17
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG21	14	0.17
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG22	19	0.17
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG21	13	0.17
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG23	13	0.17
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG22	17	0.17
(2,3836)	1:90:A:ALA:HB3	1:64:A:VAL:HG12	15	0.17
(2,3811)	1:48:A:GLU:HB2	1:49:A:VAL:HG21	11	0.17
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG11	6	0.17
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG12	6	0.17
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG13	6	0.17
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG23	7	0.17
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG22	13	0.17
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	9	0.17
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3555)	1:48:A:GLU:HG3	1:118:A:LEU:HD12	12	0.17
(2,3471)	1:118:A:LEU:HA	1:44:A:ILE:HG12	11	0.17
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	12	0.17
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	2	0.17
(2,3389)	1:41:A:TYR:HD1	1:36:A:LEU:HG	15	0.17
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	11	0.17
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	19	0.17
(2,3281)	1:72:A:LYS:H	1:71:A:ILE:HG13	16	0.17
(2,3265)	1:94:A:LEU:HD12	1:91:A:ILE:HG12	12	0.17
(2,3065)	1:70:A:PHE:HD1	1:81:A:VAL:HB	1	0.17
(2,3065)	1:70:A:PHE:HD1	1:81:A:VAL:HB	4	0.17
(2,3065)	1:70:A:PHE:HD2	1:81:A:VAL:HB	16	0.17
(2,3050)	1:142:A:HIS:HD2	1:142:A:HIS:HB3	10	0.17
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	9	0.17
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	16	0.17
(2,2960)	1:52:A:LEU:HA	1:114:A:GLU:HG3	8	0.17
(2,2960)	1:52:A:LEU:HA	1:114:A:GLU:HG3	14	0.17
(2,2874)	1:118:A:LEU:HD21	1:48:A:GLU:HG3	9	0.17
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	4	0.17
(2,2825)	1:25:A:LYS:HB3	1:26:A:ASP:HB2	3	0.17
(2,2806)	1:15:A:SER:HB3	1:38:A:ASN:HB2	10	0.17
(2,2658)	1:81:A:VAL:HG21	1:79:A:TYR:HB2	4	0.17
(2,2658)	1:81:A:VAL:HG22	1:79:A:TYR:HB2	14	0.17
(2,2634)	1:35:A:ARG:HB3	1:35:A:ARG:HD3	4	0.17
(2,2634)	1:35:A:ARG:HB2	1:35:A:ARG:HD3	5	0.17
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	5	0.17
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	10	0.17
(2,2542)	1:115:A:TYR:HD2	1:111:A:LEU:HB2	15	0.17
(2,2375)	1:104:A:LEU:HD22	1:78:A:GLU:HA	15	0.17
(2,2340)	1:114:A:GLU:HB3	1:115:A:TYR:HA	1	0.17
(2,2340)	1:114:A:GLU:HB3	1:115:A:TYR:HA	7	0.17
(2,2298)	1:3:A:ASP:HB3	1:3:A:ASP:HA	8	0.17
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	8	0.17
(2,1998)	1:115:A:TYR:HD1	1:112:A:LEU:HA	9	0.17
(2,1998)	1:115:A:TYR:HD2	1:112:A:LEU:HA	11	0.17
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	2	0.17
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	20	0.17
(2,1899)	1:76:A:ILE:HD13	1:73:A:SER:HB3	20	0.17
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB3	10	0.17
(2,1804)	1:100:A:SER:HA	1:100:A:SER:HB2	17	0.17
(2,1731)	1:56:A:ILE:HG22	1:24:A:ILE:HA	11	0.17
(2,1718)	1:64:A:VAL:HB	1:24:A:ILE:HA	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1660)	1:130:A:THR:HG22	1:132:A:GLU:H	8	0.17
(2,1654)	1:41:A:TYR:HB3	1:36:A:LEU:H	6	0.17
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	1	0.17
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	10	0.17
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	14	0.17
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	18	0.17
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	12	0.17
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	1	0.17
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	4	0.17
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	5	0.17
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	13	0.17
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	14	0.17
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	18	0.17
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	6	0.17
(2,1563)	1:69:A:ILE:HG12	1:120:A:PHE:H	10	0.17
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	13	0.17
(2,1540)	1:31:A:LYS:HB3	1:30:A:GLY:H	8	0.17
(2,1496)	1:71:A:ILE:HG12	1:83:A:GLY:H	15	0.17
(2,1496)	1:71:A:ILE:HG12	1:83:A:GLY:H	17	0.17
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	5	0.17
(2,1487)	1:95:A:LEU:HB3	1:96:A:GLY:H	13	0.17
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	2	0.17
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	4	0.17
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	20	0.17
(2,1445)	1:65:A:LYS:HG2	1:23:A:THR:H	3	0.17
(2,1389)	1:106:A:VAL:HG12	1:105:A:ASN:HD21	16	0.17
(2,1387)	1:36:A:LEU:HD13	1:16:A:SER:H	10	0.17
(2,1386)	1:65:A:LYS:HD3	1:21:A:TYR:H	2	0.17
(2,1330)	1:137:A:GLU:HG2	1:136:A:SER:H	14	0.17
(2,1244)	1:34:A:ILE:HD13	1:20:A:GLU:H	19	0.17
(2,1236)	1:19:A:ALA:HB1	1:38:A:ASN:H	8	0.17
(2,1236)	1:19:A:ALA:HB3	1:38:A:ASN:H	19	0.17
(2,1196)	1:45:A:LYS:HB2	1:47:A:ASP:H	11	0.17
(2,1188)	1:37:A:ASN:HB2	1:15:A:SER:H	6	0.17
(2,1188)	1:37:A:ASN:HB2	1:15:A:SER:H	15	0.17
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	20	0.17
(2,1104)	1:37:A:ASN:H	1:20:A:GLU:H	6	0.17
(2,1082)	1:24:A:ILE:HG23	1:25:A:LYS:H	11	0.17
(2,1082)	1:24:A:ILE:HG23	1:25:A:LYS:H	12	0.17
(2,1082)	1:24:A:ILE:HG22	1:25:A:LYS:H	20	0.17
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	15	0.17
(2,980)	1:141:A:HIS:HB2	1:141:A:HIS:H	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,968)	1:105:A:ASN:HA	1:78:A:GLU:H	6	0.17
(2,871)	1:119:A:ILE:HD11	1:119:A:ILE:H	9	0.17
(2,862)	1:111:A:LEU:HD21	1:111:A:LEU:H	10	0.17
(2,831)	1:119:A:ILE:HD11	1:112:A:LEU:H	10	0.17
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	8	0.17
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	20	0.17
(2,819)	1:112:A:LEU:HB2	1:111:A:LEU:H	19	0.17
(2,791)	1:111:A:LEU:HB3	1:112:A:LEU:H	6	0.17
(2,784)	1:61:A:TRP:HB2	1:24:A:ILE:H	2	0.17
(2,764)	1:29:A:ASP:HB3	1:28:A:LEU:H	11	0.17
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	11	0.17
(2,677)	1:78:A:GLU:HA	1:103:A:ILE:H	2	0.17
(2,677)	1:78:A:GLU:HA	1:103:A:ILE:H	10	0.17
(2,605)	1:28:A:LEU:HD21	1:51:A:LYS:H	4	0.17
(2,544)	1:10:A:LEU:HG	1:10:A:LEU:H	2	0.17
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	6	0.17
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	8	0.17
(2,348)	1:58:A:LEU:HD23	1:61:A:TRP:H	13	0.17
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	12	0.17
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	3	0.17
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	6	0.17
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	12	0.17
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	15	0.17
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	17	0.17
(2,195)	1:92:A:SER:HA	1:99:A:ILE:H	3	0.17
(2,185)	1:35:A:ARG:HE	1:36:A:LEU:H	20	0.17
(2,154)	1:71:A:ILE:HD12	1:122:A:ILE:H	8	0.17
(2,145)	1:121:A:ILE:HG13	1:70:A:PHE:H	10	0.17
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	7	0.17
(2,118)	1:124:A:SER:HB3	1:123:A:LEU:H	9	0.17
(2,108)	1:67:A:PRO:HA	1:120:A:PHE:H	11	0.17
(2,95)	1:70:A:PHE:HD1	1:122:A:ILE:H	14	0.17
(2,84)	1:24:A:ILE:HG21	1:61:A:TRP:HE1	13	0.17
(2,34)	1:71:A:ILE:HG23	1:72:A:LYS:H	2	0.17
(2,34)	1:71:A:ILE:HG23	1:72:A:LYS:H	12	0.17
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	9	0.17
(2,4705)	1:58:A:LEU:HA	1:61:A:TRP:HZ3	11	0.16
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE1	11	0.16
(2,4659)	1:41:A:TYR:HB3	1:41:A:TYR:HE2	7	0.16
(2,4659)	1:21:A:TYR:HB3	1:21:A:TYR:HE2	9	0.16
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE1	3	0.16
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE2	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE1	18	0.16
(2,4648)	1:20:A:GLU:HA	1:21:A:TYR:HE1	4	0.16
(2,4641)	1:78:A:GLU:HA	1:79:A:TYR:HE1	13	0.16
(2,4551)	1:69:A:ILE:HD12	1:120:A:PHE:HE1	7	0.16
(2,4469)	1:69:A:ILE:HD12	1:21:A:TYR:HD2	2	0.16
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	11	0.16
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	13	0.16
(2,4373)	1:130:A:THR:HG23	1:131:A:GLU:HB2	6	0.16
(2,4264)	1:51:A:LYS:HE2	1:114:A:GLU:HG2	19	0.16
(2,4243)	1:102:A:VAL:HG21	1:104:A:LEU:HA	20	0.16
(2,4225)	1:23:A:THR:HG22	1:62:A:SER:HB2	7	0.16
(2,4225)	1:23:A:THR:HG21	1:62:A:SER:HB2	10	0.16
(2,4225)	1:23:A:THR:HG21	1:62:A:SER:HB2	13	0.16
(2,4225)	1:23:A:THR:HG22	1:62:A:SER:HB2	14	0.16
(2,4225)	1:23:A:THR:HG23	1:62:A:SER:HB2	16	0.16
(2,4207)	1:70:A:PHE:HE2	1:91:A:ILE:HD11	5	0.16
(2,4207)	1:70:A:PHE:HE1	1:91:A:ILE:HD11	8	0.16
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD11	15	0.16
(2,4151)	1:44:A:ILE:HA	1:66:A:ILE:HD12	4	0.16
(2,4150)	1:17:A:SER:HB3	1:122:A:ILE:HD12	1	0.16
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD11	3	0.16
(2,4143)	1:107:A:ASP:HA	1:103:A:ILE:HD12	5	0.16
(2,4077)	1:90:A:ALA:H	1:56:A:ILE:HD13	6	0.16
(2,4012)	1:68:A:PHE:HB3	1:66:A:ILE:HG22	4	0.16
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG21	4	0.16
(2,3975)	1:111:A:LEU:HA	1:119:A:ILE:HG21	1	0.16
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG21	3	0.16
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG22	17	0.16
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG21	5	0.16
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG23	10	0.16
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG21	12	0.16
(2,3911)	1:70:A:PHE:HE1	1:103:A:ILE:HG21	2	0.16
(2,3911)	1:70:A:PHE:HE1	1:103:A:ILE:HG21	4	0.16
(2,3911)	1:70:A:PHE:HE1	1:103:A:ILE:HG22	7	0.16
(2,3908)	1:48:A:GLU:H	1:44:A:ILE:HG22	13	0.16
(2,3846)	1:103:A:ILE:HG12	1:108:A:VAL:HG23	1	0.16
(2,3836)	1:90:A:ALA:HB1	1:64:A:VAL:HG13	10	0.16
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG12	2	0.16
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG13	19	0.16
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG13	12	0.16
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG22	6	0.16
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG22	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3471)	1:118:A:LEU:HA	1:44:A:ILE:HG12	12	0.16
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	3	0.16
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	14	0.16
(2,3467)	1:52:A:LEU:HA	1:51:A:LYS:HG3	15	0.16
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	20	0.16
(2,3422)	1:71:A:ILE:HA	1:122:A:ILE:HG13	14	0.16
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	10	0.16
(2,3265)	1:94:A:LEU:HD11	1:91:A:ILE:HG12	5	0.16
(2,3085)	1:21:A:TYR:HD2	1:20:A:GLU:HB2	3	0.16
(2,3085)	1:21:A:TYR:HD1	1:20:A:GLU:HB2	4	0.16
(2,3065)	1:70:A:PHE:HD1	1:81:A:VAL:HB	2	0.16
(2,3065)	1:70:A:PHE:HD2	1:81:A:VAL:HB	3	0.16
(2,3065)	1:70:A:PHE:HD1	1:81:A:VAL:HB	6	0.16
(2,3065)	1:70:A:PHE:HD1	1:81:A:VAL:HB	8	0.16
(2,3065)	1:70:A:PHE:HD2	1:81:A:VAL:HB	14	0.16
(2,3065)	1:70:A:PHE:HD2	1:81:A:VAL:HB	17	0.16
(2,3065)	1:70:A:PHE:HD2	1:81:A:VAL:HB	20	0.16
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	2	0.16
(2,2827)	1:45:A:LYS:HB3	1:47:A:ASP:HB3	1	0.16
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	18	0.16
(2,2658)	1:81:A:VAL:HG21	1:79:A:TYR:HB2	20	0.16
(2,2634)	1:35:A:ARG:HB3	1:35:A:ARG:HD3	6	0.16
(2,2634)	1:35:A:ARG:HB3	1:35:A:ARG:HD3	15	0.16
(2,2634)	1:35:A:ARG:HB2	1:35:A:ARG:HD3	20	0.16
(2,2375)	1:104:A:LEU:HD23	1:78:A:GLU:HA	5	0.16
(2,2356)	1:19:A:ALA:HB3	1:36:A:LEU:HA	4	0.16
(2,2298)	1:3:A:ASP:HB3	1:3:A:ASP:HA	10	0.16
(2,2235)	1:95:A:LEU:H	1:90:A:ALA:HA	6	0.16
(2,2235)	1:95:A:LEU:H	1:90:A:ALA:HA	20	0.16
(2,2179)	1:108:A:VAL:HG12	1:105:A:ASN:HA	13	0.16
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	4	0.16
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	15	0.16
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	18	0.16
(2,1998)	1:115:A:TYR:HD2	1:112:A:LEU:HA	7	0.16
(2,1948)	1:92:A:SER:H	1:99:A:ILE:HA	2	0.16
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	15	0.16
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	16	0.16
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	18	0.16
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	19	0.16
(2,1904)	1:56:A:ILE:HD13	1:53:A:SER:HA	7	0.16
(2,1884)	1:44:A:ILE:HG23	1:117:A:SER:HB3	15	0.16
(2,1877)	1:137:A:GLU:HB2	1:136:A:SER:HB2	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	20	0.16
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	9	0.16
(2,1847)	1:75:A:GLU:HB2	1:73:A:SER:HB3	2	0.16
(2,1804)	1:100:A:SER:HA	1:100:A:SER:HB2	5	0.16
(2,1804)	1:100:A:SER:HA	1:100:A:SER:HB2	12	0.16
(2,1804)	1:100:A:SER:HA	1:100:A:SER:HB2	14	0.16
(2,1804)	1:100:A:SER:HA	1:100:A:SER:HB2	20	0.16
(2,1787)	1:21:A:TYR:HE1	1:17:A:SER:HB3	1	0.16
(2,1781)	1:68:A:PHE:HE1	1:91:A:ILE:HA	13	0.16
(2,1729)	1:52:A:LEU:HG	1:49:A:VAL:HA	12	0.16
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	12	0.16
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	16	0.16
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	20	0.16
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	4	0.16
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	11	0.16
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	8	0.16
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	19	0.16
(2,1611)	1:86:A:TRP:HD1	1:84:A:GLU:H	14	0.16
(2,1599)	1:62:A:SER:HA	1:26:A:ASP:H	15	0.16
(2,1595)	1:95:A:LEU:HD13	1:107:A:ASP:H	10	0.16
(2,1571)	1:30:A:GLY:H	1:32:A:LEU:H	13	0.16
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	3	0.16
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	15	0.16
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	17	0.16
(2,1556)	1:33:A:LYS:HB2	1:43:A:GLU:H	1	0.16
(2,1496)	1:71:A:ILE:HG12	1:83:A:GLY:H	2	0.16
(2,1471)	1:87:A:ASN:HB3	1:83:A:GLY:H	10	0.16
(2,1460)	1:9:A:GLY:HA3	1:9:A:GLY:H	3	0.16
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	9	0.16
(2,1330)	1:137:A:GLU:HG2	1:136:A:SER:H	4	0.16
(2,1324)	1:100:A:SER:HB3	1:101:A:ASN:HD22	20	0.16
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	10	0.16
(2,1244)	1:34:A:ILE:HD13	1:20:A:GLU:H	4	0.16
(2,1222)	1:33:A:LYS:HD3	1:41:A:TYR:H	20	0.16
(2,1180)	1:45:A:LYS:HE3	1:47:A:ASP:H	17	0.16
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	2	0.16
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	5	0.16
(2,1063)	1:23:A:THR:HG23	1:25:A:LYS:H	3	0.16
(2,1063)	1:23:A:THR:HG22	1:25:A:LYS:H	6	0.16
(2,1063)	1:23:A:THR:HG22	1:25:A:LYS:H	20	0.16
(2,1030)	1:22:A:VAL:HB	1:29:A:ASP:H	13	0.16
(2,1030)	1:22:A:VAL:HB	1:29:A:ASP:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,962)	1:95:A:LEU:HA	1:97:A:ARG:H	10	0.16
(2,962)	1:95:A:LEU:HA	1:97:A:ARG:H	11	0.16
(2,962)	1:95:A:LEU:HA	1:97:A:ARG:H	19	0.16
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	7	0.16
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	11	0.16
(2,895)	1:91:A:ILE:HD12	1:88:A:LYS:H	2	0.16
(2,885)	1:66:A:ILE:HD13	1:26:A:ASP:H	7	0.16
(2,871)	1:119:A:ILE:HD12	1:119:A:ILE:H	6	0.16
(2,871)	1:119:A:ILE:HD13	1:119:A:ILE:H	19	0.16
(2,862)	1:95:A:LEU:HD23	1:111:A:LEU:H	5	0.16
(2,862)	1:111:A:LEU:HD23	1:111:A:LEU:H	14	0.16
(2,844)	1:94:A:LEU:HD21	1:94:A:LEU:H	1	0.16
(2,831)	1:119:A:ILE:HD11	1:112:A:LEU:H	5	0.16
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	17	0.16
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	6	0.16
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	14	0.16
(2,819)	1:110:A:LYS:HD2	1:111:A:LEU:H	18	0.16
(2,816)	1:51:A:LYS:HG2	1:49:A:VAL:H	5	0.16
(2,816)	1:51:A:LYS:HG2	1:49:A:VAL:H	8	0.16
(2,816)	1:51:A:LYS:HG2	1:49:A:VAL:H	16	0.16
(2,791)	1:111:A:LEU:HB3	1:112:A:LEU:H	10	0.16
(2,764)	1:29:A:ASP:HB3	1:28:A:LEU:H	8	0.16
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	4	0.16
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	5	0.16
(2,677)	1:78:A:GLU:HA	1:103:A:ILE:H	19	0.16
(2,663)	1:115:A:TYR:HD2	1:112:A:LEU:H	4	0.16
(2,580)	1:52:A:LEU:HG	1:51:A:LYS:H	7	0.16
(2,571)	1:118:A:LEU:HD13	1:52:A:LEU:H	17	0.16
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	1	0.16
(2,544)	1:10:A:LEU:HG	1:10:A:LEU:H	10	0.16
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	18	0.16
(2,348)	1:58:A:LEU:HD23	1:61:A:TRP:H	8	0.16
(2,348)	1:58:A:LEU:HD22	1:61:A:TRP:H	15	0.16
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	8	0.16
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	9	0.16
(2,166)	1:22:A:VAL:HG11	1:31:A:LYS:H	5	0.16
(2,166)	1:22:A:VAL:HG12	1:31:A:LYS:H	5	0.16
(2,166)	1:22:A:VAL:HG13	1:31:A:LYS:H	5	0.16
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	18	0.16
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	11	0.16
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	12	0.16
(2,123)	1:28:A:LEU:HA	1:31:A:LYS:H	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,123)	1:28:A:LEU:HA	1:31:A:LYS:H	13	0.16
(2,84)	1:24:A:ILE:HG23	1:61:A:TRP:HE1	2	0.16
(2,84)	1:24:A:ILE:HG23	1:61:A:TRP:HE1	17	0.16
(2,4667)	1:111:A:LEU:HD23	1:115:A:TYR:HE2	18	0.15
(2,4661)	1:57:A:PRO:HG2	1:59:A:TYR:HE1	9	0.15
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE1	4	0.15
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE2	20	0.15
(2,4505)	1:122:A:ILE:HD11	1:14:A:PHE:HD2	18	0.15
(2,4450)	1:132:A:GLU:HB2	1:129:A:TYR:HD1	7	0.15
(2,4415)	1:134:A:GLU:HB3	1:133:A:THR:HB	4	0.15
(2,4398)	1:52:A:LEU:HA	1:55:A:ARG:HD2	8	0.15
(2,4398)	1:52:A:LEU:HA	1:55:A:ARG:HD3	15	0.15
(2,4385)	1:46:A:LYS:HE2	1:50:A:GLU:HG2	3	0.15
(2,4385)	1:129:A:TYR:HB3	1:131:A:GLU:HG3	5	0.15
(2,4291)	1:52:A:LEU:HG	1:94:A:LEU:HD13	20	0.15
(2,4225)	1:23:A:THR:HG22	1:62:A:SER:HB2	6	0.15
(2,4225)	1:23:A:THR:HG21	1:62:A:SER:HB2	15	0.15
(2,4225)	1:23:A:THR:HG23	1:62:A:SER:HB2	17	0.15
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD13	11	0.15
(2,4092)	1:14:A:PHE:HD2	1:122:A:ILE:HD11	18	0.15
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	7	0.15
(2,4012)	1:68:A:PHE:HB3	1:66:A:ILE:HG22	6	0.15
(2,4011)	1:68:A:PHE:HB3	1:119:A:ILE:HG22	14	0.15
(2,4006)	1:87:A:ASN:HB3	1:99:A:ILE:HG22	3	0.15
(2,4000)	1:72:A:LYS:HE3	1:121:A:ILE:HG21	7	0.15
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG23	2	0.15
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG22	7	0.15
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG23	16	0.15
(2,3971)	1:116:A:THR:HA	1:119:A:ILE:HG23	3	0.15
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG22	6	0.15
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG21	1	0.15
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB3	15	0.15
(2,3836)	1:90:A:ALA:HB3	1:64:A:VAL:HG13	12	0.15
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG11	4	0.15
(2,3803)	1:42:A:HIS:HB2	1:36:A:LEU:HD22	1	0.15
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG23	15	0.15
(2,3720)	1:86:A:TRP:HH2	1:63:A:LEU:HD22	7	0.15
(2,3703)	1:119:A:ILE:H	1:112:A:LEU:HD23	5	0.15
(2,3672)	1:79:A:TYR:H	1:102:A:VAL:HG11	10	0.15
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	6	0.15
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	7	0.15
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG23	2	0.15
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	11	0.15
(2,3462)	1:135:A:LEU:HA	1:135:A:LEU:HG	17	0.15
(2,3435)	1:23:A:THR:HB	1:65:A:LYS:HG3	3	0.15
(2,3409)	1:79:A:TYR:HD1	1:123:A:LEU:HD21	11	0.15
(2,3405)	1:115:A:TYR:HE1	1:118:A:LEU:HD13	11	0.15
(2,3389)	1:41:A:TYR:HD2	1:36:A:LEU:HG	8	0.15
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	4	0.15
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	17	0.15
(2,3281)	1:72:A:LYS:H	1:71:A:ILE:HG13	10	0.15
(2,3265)	1:94:A:LEU:HD13	1:91:A:ILE:HG12	4	0.15
(2,3108)	1:42:A:HIS:HA	1:43:A:GLU:HB2	10	0.15
(2,3065)	1:70:A:PHE:HD2	1:81:A:VAL:HB	5	0.15
(2,3065)	1:70:A:PHE:HD1	1:81:A:VAL:HB	19	0.15
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	6	0.15
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	7	0.15
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	20	0.15
(2,2973)	1:109:A:GLU:HA	1:109:A:GLU:HG2	11	0.15
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	10	0.15
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	1	0.15
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	5	0.15
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	8	0.15
(2,2806)	1:15:A:SER:HB3	1:38:A:ASN:HB2	14	0.15
(2,2652)	1:95:A:LEU:HD23	1:107:A:ASP:HB2	20	0.15
(2,2634)	1:35:A:ARG:HB2	1:35:A:ARG:HD3	10	0.15
(2,2634)	1:35:A:ARG:HB3	1:35:A:ARG:HD3	19	0.15
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	14	0.15
(2,2538)	1:115:A:TYR:HD1	1:118:A:LEU:HB3	6	0.15
(2,2489)	1:95:A:LEU:HB3	1:96:A:GLY:HA3	1	0.15
(2,2466)	1:69:A:ILE:HG23	1:70:A:PHE:HA	13	0.15
(2,2466)	1:69:A:ILE:HG22	1:70:A:PHE:HA	15	0.15
(2,2466)	1:69:A:ILE:HG23	1:70:A:PHE:HA	17	0.15
(2,2298)	1:3:A:ASP:HB3	1:3:A:ASP:HA	12	0.15
(2,2298)	1:3:A:ASP:HB3	1:3:A:ASP:HA	17	0.15
(2,2235)	1:95:A:LEU:H	1:90:A:ALA:HA	14	0.15
(2,2235)	1:95:A:LEU:H	1:90:A:ALA:HA	19	0.15
(2,2131)	1:85:A:GLN:HG2	1:86:A:TRP:HA	17	0.15
(2,2099)	1:134:A:GLU:HG2	1:131:A:GLU:HA	20	0.15
(2,2046)	1:91:A:ILE:HA	1:88:A:LYS:HA	6	0.15
(2,1998)	1:115:A:TYR:HD2	1:112:A:LEU:HA	6	0.15
(2,1948)	1:92:A:SER:H	1:99:A:ILE:HA	3	0.15
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	13	0.15
(2,1828)	1:125:A:PRO:HB2	1:125:A:PRO:HA	6	0.15
(2,1828)	1:125:A:PRO:HB2	1:125:A:PRO:HA	16	0.15
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB3	14	0.15
(2,1819)	1:105:A:ASN:HB3	1:106:A:VAL:HA	12	0.15
(2,1781)	1:68:A:PHE:HE2	1:91:A:ILE:HA	5	0.15
(2,1735)	1:119:A:ILE:HG23	1:116:A:THR:HA	3	0.15
(2,1731)	1:56:A:ILE:HG21	1:24:A:ILE:HA	7	0.15
(2,1731)	1:56:A:ILE:HG21	1:24:A:ILE:HA	14	0.15
(2,1721)	1:134:A:GLU:HB2	1:133:A:THR:HB	7	0.15
(2,1717)	1:49:A:VAL:HB	1:24:A:ILE:HA	17	0.15
(2,1654)	1:41:A:TYR:HB3	1:36:A:LEU:H	1	0.15
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	3	0.15
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	4	0.15
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	6	0.15
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	13	0.15
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	14	0.15
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	15	0.15
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	11	0.15
(2,1599)	1:62:A:SER:HA	1:26:A:ASP:H	5	0.15
(2,1571)	1:30:A:GLY:H	1:32:A:LEU:H	4	0.15
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	4	0.15
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	6	0.15
(2,1562)	1:122:A:ILE:HG13	1:123:A:LEU:H	20	0.15
(2,1509)	1:59:A:TYR:HA	1:62:A:SER:H	14	0.15
(2,1499)	1:93:A:ILE:HG21	1:96:A:GLY:H	9	0.15
(2,1496)	1:71:A:ILE:HG12	1:83:A:GLY:H	4	0.15
(2,1460)	1:9:A:GLY:HA3	1:9:A:GLY:H	12	0.15
(2,1447)	1:22:A:VAL:HG21	1:23:A:THR:H	20	0.15
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	3	0.15
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	5	0.15
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	10	0.15
(2,1388)	1:34:A:ILE:HG22	1:21:A:TYR:H	4	0.15
(2,1388)	1:34:A:ILE:HG23	1:21:A:TYR:H	17	0.15
(2,1387)	1:36:A:LEU:HD11	1:16:A:SER:H	4	0.15
(2,1350)	1:50:A:GLU:HB3	1:53:A:SER:H	14	0.15
(2,1330)	1:137:A:GLU:HG2	1:136:A:SER:H	2	0.15
(2,1313)	1:14:A:PHE:HB2	1:16:A:SER:H	19	0.15
(2,1310)	1:125:A:PRO:HD2	1:126:A:THR:H	19	0.15
(2,1310)	1:125:A:PRO:HD3	1:126:A:THR:H	19	0.15
(2,1255)	1:52:A:LEU:HD12	1:54:A:SER:H	20	0.15
(2,1248)	1:94:A:LEU:HD12	1:95:A:LEU:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1167)	1:128:A:SER:HB3	1:128:A:SER:H	7	0.15
(2,1066)	1:99:A:ILE:HD11	1:97:A:ARG:H	12	0.15
(2,1025)	1:118:A:LEU:HB2	1:115:A:TYR:H	1	0.15
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	4	0.15
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	9	0.15
(2,980)	1:141:A:HIS:HB2	1:141:A:HIS:H	5	0.15
(2,886)	1:24:A:ILE:HG22	1:26:A:ASP:H	5	0.15
(2,871)	1:119:A:ILE:HD12	1:119:A:ILE:H	8	0.15
(2,871)	1:119:A:ILE:HD13	1:119:A:ILE:H	18	0.15
(2,862)	1:111:A:LEU:HD21	1:111:A:LEU:H	9	0.15
(2,841)	1:5:A:ILE:HD12	1:5:A:ILE:H	14	0.15
(2,831)	1:119:A:ILE:HD12	1:112:A:LEU:H	15	0.15
(2,822)	1:88:A:LYS:HD3	1:88:A:LYS:H	1	0.15
(2,819)	1:112:A:LEU:HB2	1:111:A:LEU:H	5	0.15
(2,819)	1:110:A:LYS:HD2	1:111:A:LEU:H	10	0.15
(2,816)	1:51:A:LYS:HG2	1:49:A:VAL:H	2	0.15
(2,784)	1:61:A:TRP:HB2	1:24:A:ILE:H	18	0.15
(2,605)	1:28:A:LEU:HD23	1:51:A:LYS:H	18	0.15
(2,575)	1:104:A:LEU:HD21	1:105:A:ASN:H	13	0.15
(2,575)	1:104:A:LEU:HD22	1:105:A:ASN:H	13	0.15
(2,575)	1:104:A:LEU:HD23	1:105:A:ASN:H	13	0.15
(2,571)	1:118:A:LEU:HD13	1:52:A:LEU:H	9	0.15
(2,568)	1:49:A:VAL:HG11	1:50:A:GLU:H	10	0.15
(2,568)	1:49:A:VAL:HG12	1:50:A:GLU:H	10	0.15
(2,568)	1:49:A:VAL:HG13	1:50:A:GLU:H	10	0.15
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	11	0.15
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	16	0.15
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	3	0.15
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	5	0.15
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	17	0.15
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	20	0.15
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	7	0.15
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	19	0.15
(2,225)	1:98:A:GLU:HG2	1:99:A:ILE:H	11	0.15
(2,225)	1:98:A:GLU:HG3	1:99:A:ILE:H	18	0.15
(2,205)	1:90:A:ALA:HA	1:93:A:ILE:H	14	0.15
(2,154)	1:71:A:ILE:HD13	1:122:A:ILE:H	14	0.15
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	15	0.15
(2,123)	1:28:A:LEU:HA	1:31:A:LYS:H	3	0.15
(2,123)	1:28:A:LEU:HA	1:31:A:LYS:H	4	0.15
(2,123)	1:28:A:LEU:HA	1:31:A:LYS:H	19	0.15
(2,100)	1:79:A:TYR:HE2	1:70:A:PHE:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:71:A:ILE:HG23	1:72:A:LYS:H	9	0.15
(2,34)	1:71:A:ILE:HG23	1:72:A:LYS:H	18	0.15
(2,29)	1:48:A:GLU:HG3	1:46:A:LYS:H	7	0.15
(2,29)	1:48:A:GLU:HG3	1:46:A:LYS:H	18	0.15
(2,9)	1:85:A:GLN:HB3	1:86:A:TRP:HE1	20	0.15
(2,4705)	1:58:A:LEU:HA	1:61:A:TRP:HZ3	10	0.14
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE1	15	0.14
(2,4667)	1:123:A:LEU:HD21	1:79:A:TYR:HE2	13	0.14
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE1	2	0.14
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE2	17	0.14
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE2	19	0.14
(2,4644)	1:123:A:LEU:HA	1:79:A:TYR:HE2	20	0.14
(2,4474)	1:36:A:LEU:HD21	1:41:A:TYR:HD1	19	0.14
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	14	0.14
(2,4438)	1:18:A:PRO:HD3	1:21:A:TYR:HD1	7	0.14
(2,4303)	1:89:A:LYS:HD2	1:63:A:LEU:HD11	1	0.14
(2,4282)	1:138:A:MET:HA	1:141:A:HIS:HB3	19	0.14
(2,4253)	1:27:A:ALA:HB2	1:26:A:ASP:HB2	1	0.14
(2,4243)	1:102:A:VAL:HG21	1:104:A:LEU:HA	11	0.14
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD13	19	0.14
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG22	17	0.14
(2,4093)	1:120:A:PHE:HD2	1:122:A:ILE:HD12	8	0.14
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD12	3	0.14
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD12	6	0.14
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD13	9	0.14
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	16	0.14
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD13	20	0.14
(2,4011)	1:68:A:PHE:HB3	1:119:A:ILE:HG21	12	0.14
(2,4004)	1:26:A:ASP:HB3	1:22:A:VAL:HG21	10	0.14
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG23	12	0.14
(2,3938)	1:80:A:PHE:HA	1:71:A:ILE:HG21	14	0.14
(2,3908)	1:48:A:GLU:H	1:44:A:ILE:HG21	15	0.14
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG12	10	0.14
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG13	18	0.14
(2,3632)	1:103:A:ILE:HG23	1:95:A:LEU:HG	10	0.14
(2,3632)	1:94:A:LEU:HD13	1:95:A:LEU:HG	11	0.14
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	3	0.14
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	10	0.14
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	15	0.14
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	17	0.14
(2,3606)	1:56:A:ILE:HG13	1:57:A:PRO:HG3	19	0.14
(2,3587)	1:89:A:LYS:HB3	1:64:A:VAL:HG22	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3471)	1:32:A:LEU:HA	1:44:A:ILE:HG13	6	0.14
(2,3434)	1:33:A:LYS:HA	1:34:A:ILE:HG12	4	0.14
(2,3389)	1:41:A:TYR:HD1	1:36:A:LEU:HG	6	0.14
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	6	0.14
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	8	0.14
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	9	0.14
(2,3271)	1:58:A:LEU:HD22	1:25:A:LYS:HD2	18	0.14
(2,3271)	1:58:A:LEU:HD21	1:25:A:LYS:HD2	20	0.14
(2,3247)	1:60:A:LEU:HD21	1:89:A:LYS:HB3	14	0.14
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	7	0.14
(2,3065)	1:70:A:PHE:HD1	1:81:A:VAL:HB	7	0.14
(2,3065)	1:70:A:PHE:HD2	1:81:A:VAL:HB	13	0.14
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	3	0.14
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	10	0.14
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	15	0.14
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	17	0.14
(2,2960)	1:52:A:LEU:HA	1:114:A:GLU:HG3	5	0.14
(2,2960)	1:52:A:LEU:HA	1:114:A:GLU:HG3	10	0.14
(2,2954)	1:137:A:GLU:HA	1:137:A:GLU:HG2	16	0.14
(2,2874)	1:118:A:LEU:HD22	1:48:A:GLU:HG3	5	0.14
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	4	0.14
(2,2658)	1:81:A:VAL:HG23	1:79:A:TYR:HB2	12	0.14
(2,2653)	1:95:A:LEU:HD12	1:107:A:ASP:HB2	19	0.14
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	4	0.14
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	8	0.14
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	10	0.14
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	15	0.14
(2,2466)	1:69:A:ILE:HG22	1:70:A:PHE:HA	7	0.14
(2,2372)	1:34:A:ILE:HG21	1:21:A:TYR:HA	7	0.14
(2,2356)	1:19:A:ALA:HB1	1:36:A:LEU:HA	14	0.14
(2,2340)	1:114:A:GLU:HB3	1:115:A:TYR:HA	16	0.14
(2,2318)	1:50:A:GLU:HB2	1:47:A:ASP:HA	12	0.14
(2,2318)	1:110:A:LYS:HB2	1:107:A:ASP:HA	16	0.14
(2,2298)	1:3:A:ASP:HB3	1:3:A:ASP:HA	3	0.14
(2,2235)	1:95:A:LEU:H	1:90:A:ALA:HA	11	0.14
(2,2179)	1:108:A:VAL:HG12	1:105:A:ASN:HA	8	0.14
(2,2179)	1:108:A:VAL:HG13	1:105:A:ASN:HA	11	0.14
(2,2175)	1:94:A:LEU:HD21	1:52:A:LEU:HA	19	0.14
(2,2163)	1:102:A:VAL:HG21	1:103:A:ILE:HA	19	0.14
(2,2145)	1:46:A:LYS:HD2	1:46:A:LYS:HA	16	0.14
(2,2143)	1:133:A:THR:HG22	1:134:A:GLU:HA	18	0.14
(2,2084)	1:31:A:LYS:HB3	1:22:A:VAL:HA	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2074)	1:61:A:TRP:HB2	1:25:A:LYS:HA	4	0.14
(2,2030)	1:32:A:LEU:HA	1:46:A:LYS:HA	5	0.14
(2,1998)	1:115:A:TYR:HD1	1:112:A:LEU:HA	12	0.14
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	4	0.14
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	10	0.14
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	11	0.14
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	13	0.14
(2,1731)	1:56:A:ILE:HG21	1:24:A:ILE:HA	4	0.14
(2,1731)	1:56:A:ILE:HG22	1:24:A:ILE:HA	8	0.14
(2,1717)	1:49:A:VAL:HB	1:24:A:ILE:HA	16	0.14
(2,1654)	1:41:A:TYR:HB3	1:36:A:LEU:H	18	0.14
(2,1654)	1:41:A:TYR:HB3	1:36:A:LEU:H	19	0.14
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	7	0.14
(2,1646)	1:88:A:LYS:HB2	1:87:A:ASN:H	11	0.14
(2,1626)	1:135:A:LEU:HD22	1:136:A:SER:H	1	0.14
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	8	0.14
(2,1620)	1:66:A:ILE:HB	1:66:A:ILE:H	12	0.14
(2,1523)	1:63:A:LEU:HG	1:62:A:SER:H	10	0.14
(2,1499)	1:93:A:ILE:HG21	1:96:A:GLY:H	7	0.14
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	12	0.14
(2,1330)	1:132:A:GLU:HG2	1:136:A:SER:H	17	0.14
(2,1238)	1:114:A:GLU:HB3	1:113:A:ARG:H	11	0.14
(2,1229)	1:130:A:THR:HG21	1:130:A:THR:H	1	0.14
(2,1229)	1:130:A:THR:HG22	1:130:A:THR:H	1	0.14
(2,1229)	1:130:A:THR:HG23	1:130:A:THR:H	1	0.14
(2,1191)	1:131:A:GLU:HG2	1:133:A:THR:H	15	0.14
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	8	0.14
(2,1030)	1:22:A:VAL:HB	1:29:A:ASP:H	16	0.14
(2,980)	1:141:A:HIS:HB2	1:141:A:HIS:H	3	0.14
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	13	0.14
(2,895)	1:91:A:ILE:HD13	1:88:A:LYS:H	4	0.14
(2,886)	1:28:A:LEU:HD11	1:26:A:ASP:H	20	0.14
(2,885)	1:66:A:ILE:HD13	1:26:A:ASP:H	18	0.14
(2,871)	1:119:A:ILE:HD12	1:119:A:ILE:H	15	0.14
(2,862)	1:111:A:LEU:HD22	1:111:A:LEU:H	11	0.14
(2,844)	1:94:A:LEU:HD23	1:94:A:LEU:H	11	0.14
(2,844)	1:94:A:LEU:HD23	1:94:A:LEU:H	14	0.14
(2,844)	1:94:A:LEU:HD23	1:94:A:LEU:H	16	0.14
(2,841)	1:5:A:ILE:HD11	1:5:A:ILE:H	19	0.14
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	12	0.14
(2,807)	1:11:A:LYS:HB2	1:12:A:ASP:H	18	0.14
(2,807)	1:11:A:LYS:HB3	1:12:A:ASP:H	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,791)	1:111:A:LEU:HB3	1:112:A:LEU:H	20	0.14
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	5	0.14
(2,764)	1:29:A:ASP:HB3	1:28:A:LEU:H	2	0.14
(2,744)	1:86:A:TRP:HB2	1:87:A:ASN:H	3	0.14
(2,663)	1:115:A:TYR:HD2	1:112:A:LEU:H	2	0.14
(2,605)	1:28:A:LEU:HD23	1:51:A:LYS:H	12	0.14
(2,605)	1:28:A:LEU:HD22	1:51:A:LYS:H	14	0.14
(2,605)	1:28:A:LEU:HD22	1:51:A:LYS:H	16	0.14
(2,582)	1:56:A:ILE:HG13	1:55:A:ARG:H	19	0.14
(2,568)	1:49:A:VAL:HG11	1:50:A:GLU:H	17	0.14
(2,568)	1:49:A:VAL:HG12	1:50:A:GLU:H	17	0.14
(2,568)	1:49:A:VAL:HG13	1:50:A:GLU:H	17	0.14
(2,554)	1:71:A:ILE:HG22	1:80:A:PHE:H	3	0.14
(2,554)	1:71:A:ILE:HG23	1:80:A:PHE:H	12	0.14
(2,554)	1:71:A:ILE:HG21	1:80:A:PHE:H	17	0.14
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	1	0.14
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	17	0.14
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	10	0.14
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	3	0.14
(2,396)	1:120:A:PHE:HE2	1:68:A:PHE:H	14	0.14
(2,348)	1:58:A:LEU:HD23	1:61:A:TRP:H	1	0.14
(2,346)	1:24:A:ILE:HD11	1:61:A:TRP:H	6	0.14
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	2	0.14
(2,332)	1:71:A:ILE:HD13	1:71:A:ILE:H	1	0.14
(2,294)	1:127:A:ARG:HA	1:127:A:ARG:H	6	0.14
(2,293)	1:129:A:TYR:HA	1:129:A:TYR:H	14	0.14
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	4	0.14
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	16	0.14
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	18	0.14
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	19	0.14
(2,185)	1:35:A:ARG:HE	1:36:A:LEU:H	5	0.14
(2,156)	1:69:A:ILE:HD12	1:120:A:PHE:H	18	0.14
(2,108)	1:67:A:PRO:HA	1:120:A:PHE:H	15	0.14
(2,100)	1:79:A:TYR:HE1	1:70:A:PHE:H	8	0.14
(2,95)	1:70:A:PHE:HD2	1:122:A:ILE:H	1	0.14
(2,95)	1:70:A:PHE:HD1	1:122:A:ILE:H	3	0.14
(2,67)	1:41:A:TYR:HB2	1:43:A:GLU:H	3	0.14
(2,33)	1:46:A:LYS:HD3	1:46:A:LYS:H	8	0.14
(2,29)	1:48:A:GLU:HG3	1:46:A:LYS:H	2	0.14
(2,29)	1:48:A:GLU:HG3	1:46:A:LYS:H	11	0.14
(2,29)	1:48:A:GLU:HG3	1:46:A:LYS:H	20	0.14
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE1	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4663)	1:114:A:GLU:HG3	1:115:A:TYR:HE2	20	0.13
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE1	2	0.13
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE1	4	0.13
(2,4660)	1:41:A:TYR:HB2	1:41:A:TYR:HE2	10	0.13
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE2	20	0.13
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE1	1	0.13
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE1	5	0.13
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE2	6	0.13
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE2	7	0.13
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE1	8	0.13
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE2	13	0.13
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE2	14	0.13
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE1	15	0.13
(2,4648)	1:20:A:GLU:HA	1:21:A:TYR:HE2	13	0.13
(2,4644)	1:123:A:LEU:HA	1:79:A:TYR:HE1	8	0.13
(2,4551)	1:122:A:ILE:HD13	1:120:A:PHE:HE2	2	0.13
(2,4457)	1:20:A:GLU:HG3	1:41:A:TYR:HD1	13	0.13
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	14	0.13
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	19	0.13
(2,4398)	1:113:A:ARG:HA	1:113:A:ARG:HD2	16	0.13
(2,4396)	1:15:A:SER:HB2	1:12:A:ASP:HB3	7	0.13
(2,4396)	1:15:A:SER:HB3	1:12:A:ASP:HB3	7	0.13
(2,4385)	1:46:A:LYS:HE2	1:50:A:GLU:HG2	19	0.13
(2,4324)	1:91:A:ILE:H	1:56:A:ILE:HD13	2	0.13
(2,4320)	1:24:A:ILE:HB	1:66:A:ILE:HG22	16	0.13
(2,4291)	1:52:A:LEU:HG	1:94:A:LEU:HD13	12	0.13
(2,4291)	1:52:A:LEU:HG	1:94:A:LEU:HD13	16	0.13
(2,4279)	1:68:A:PHE:HD1	1:118:A:LEU:HD12	17	0.13
(2,4207)	1:70:A:PHE:HE1	1:91:A:ILE:HD12	7	0.13
(2,4207)	1:70:A:PHE:HE1	1:91:A:ILE:HD11	19	0.13
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD12	7	0.13
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD13	15	0.13
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD13	17	0.13
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD11	18	0.13
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD12	18	0.13
(2,4146)	1:82:A:SER:HB2	1:71:A:ILE:HD13	18	0.13
(2,4143)	1:81:A:VAL:HA	1:103:A:ILE:HD13	9	0.13
(2,4077)	1:90:A:ALA:H	1:56:A:ILE:HD11	15	0.13
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD12	19	0.13
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG21	19	0.13
(2,4020)	1:49:A:VAL:HB	1:44:A:ILE:HG21	7	0.13
(2,4020)	1:118:A:LEU:HB3	1:44:A:ILE:HG23	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4012)	1:68:A:PHE:HB3	1:66:A:ILE:HG23	11	0.13
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG21	13	0.13
(2,3971)	1:116:A:THR:HA	1:119:A:ILE:HG21	20	0.13
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG23	1	0.13
(2,3940)	1:102:A:VAL:HA	1:102:A:VAL:HG23	16	0.13
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG21	2	0.13
(2,3925)	1:42:A:HIS:HD2	1:34:A:ILE:HG21	4	0.13
(2,3908)	1:48:A:GLU:H	1:44:A:ILE:HG21	17	0.13
(2,3836)	1:90:A:ALA:HB3	1:64:A:VAL:HG11	19	0.13
(2,3826)	1:79:A:TYR:HB2	1:108:A:VAL:HG13	9	0.13
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG11	19	0.13
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG12	19	0.13
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG13	19	0.13
(2,3784)	1:28:A:LEU:HA	1:32:A:LEU:HD21	7	0.13
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD21	7	0.13
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD22	7	0.13
(2,3730)	1:42:A:HIS:HD2	1:32:A:LEU:HD23	7	0.13
(2,3714)	1:49:A:VAL:H	1:28:A:LEU:HD21	15	0.13
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG13	10	0.13
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	2	0.13
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	13	0.13
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	18	0.13
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	19	0.13
(2,3614)	1:60:A:LEU:HB2	1:64:A:VAL:HG21	11	0.13
(2,3614)	1:60:A:LEU:HB2	1:64:A:VAL:HG22	19	0.13
(2,3555)	1:48:A:GLU:HG3	1:118:A:LEU:HD12	8	0.13
(2,3501)	1:82:A:SER:HB3	1:122:A:ILE:HG13	13	0.13
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD12	16	0.13
(2,3389)	1:21:A:TYR:HD1	1:69:A:ILE:HG13	13	0.13
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	1	0.13
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	20	0.13
(2,3281)	1:72:A:LYS:H	1:71:A:ILE:HG13	3	0.13
(2,3271)	1:58:A:LEU:HD21	1:25:A:LYS:HD2	19	0.13
(2,3265)	1:94:A:LEU:HD13	1:91:A:ILE:HG12	3	0.13
(2,3108)	1:42:A:HIS:HA	1:43:A:GLU:HB2	18	0.13
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	2	0.13
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	13	0.13
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	18	0.13
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	19	0.13
(2,2973)	1:109:A:GLU:HA	1:109:A:GLU:HG2	13	0.13
(2,2954)	1:137:A:GLU:HA	1:137:A:GLU:HG2	2	0.13
(2,2865)	1:76:A:ILE:HG23	1:105:A:ASN:HB2	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2845)	1:51:A:LYS:HG2	1:47:A:ASP:HB2	16	0.13
(2,2827)	1:45:A:LYS:HB3	1:47:A:ASP:HB3	10	0.13
(2,2806)	1:15:A:SER:HB2	1:38:A:ASN:HB2	11	0.13
(2,2605)	1:87:A:ASN:HB3	1:83:A:GLY:HA2	13	0.13
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	1	0.13
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	11	0.13
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	13	0.13
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	16	0.13
(2,2548)	1:60:A:LEU:H	1:58:A:LEU:HB2	14	0.13
(2,2496)	1:32:A:LEU:HB2	1:30:A:GLY:HA2	19	0.13
(2,2494)	1:10:A:LEU:HG	1:9:A:GLY:HA2	18	0.13
(2,2356)	1:19:A:ALA:HB1	1:36:A:LEU:HA	1	0.13
(2,2338)	1:65:A:LYS:HD2	1:21:A:TYR:HA	16	0.13
(2,2318)	1:50:A:GLU:HB2	1:47:A:ASP:HA	6	0.13
(2,2318)	1:50:A:GLU:HB2	1:47:A:ASP:HA	19	0.13
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	1	0.13
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	13	0.13
(2,2115)	1:33:A:LYS:HG3	1:41:A:TYR:HA	11	0.13
(2,2046)	1:91:A:ILE:HA	1:88:A:LYS:HA	7	0.13
(2,1948)	1:92:A:SER:H	1:99:A:ILE:HA	1	0.13
(2,1948)	1:92:A:SER:H	1:99:A:ILE:HA	15	0.13
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	3	0.13
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	8	0.13
(2,1884)	1:44:A:ILE:HG21	1:117:A:SER:HB3	13	0.13
(2,1866)	1:139:A:LEU:HB2	1:136:A:SER:HB2	11	0.13
(2,1856)	1:99:A:ILE:HG12	1:92:A:SER:HB3	6	0.13
(2,1828)	1:125:A:PRO:HB2	1:125:A:PRO:HA	8	0.13
(2,1821)	1:38:A:ASN:HB2	1:15:A:SER:HB2	11	0.13
(2,1819)	1:105:A:ASN:HB2	1:106:A:VAL:HA	8	0.13
(2,1819)	1:105:A:ASN:HB2	1:106:A:VAL:HA	9	0.13
(2,1735)	1:119:A:ILE:HG21	1:116:A:THR:HA	20	0.13
(2,1731)	1:56:A:ILE:HG22	1:24:A:ILE:HA	9	0.13
(2,1718)	1:64:A:VAL:HB	1:24:A:ILE:HA	6	0.13
(2,1627)	1:135:A:LEU:HD11	1:133:A:THR:H	5	0.13
(2,1627)	1:135:A:LEU:HD12	1:133:A:THR:H	5	0.13
(2,1627)	1:135:A:LEU:HD13	1:133:A:THR:H	5	0.13
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	10	0.13
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	17	0.13
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	19	0.13
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	20	0.13
(2,1611)	1:86:A:TRP:HD1	1:84:A:GLU:H	15	0.13
(2,1601)	1:43:A:GLU:HG3	1:34:A:ILE:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1523)	1:63:A:LEU:HG	1:62:A:SER:H	12	0.13
(2,1523)	1:63:A:LEU:HG	1:62:A:SER:H	18	0.13
(2,1499)	1:93:A:ILE:HG23	1:96:A:GLY:H	8	0.13
(2,1496)	1:71:A:ILE:HG12	1:83:A:GLY:H	16	0.13
(2,1460)	1:9:A:GLY:HA3	1:9:A:GLY:H	13	0.13
(2,1424)	1:25:A:LYS:HA	1:23:A:THR:H	8	0.13
(2,1404)	1:122:A:ILE:HD12	1:37:A:ASN:HD22	15	0.13
(2,1388)	1:34:A:ILE:HG22	1:21:A:TYR:H	5	0.13
(2,1388)	1:22:A:VAL:HG13	1:21:A:TYR:H	6	0.13
(2,1306)	1:15:A:SER:HA	1:37:A:ASN:HD22	7	0.13
(2,1306)	1:19:A:ALA:HA	1:37:A:ASN:HD22	10	0.13
(2,1273)	1:115:A:TYR:HD2	1:53:A:SER:H	8	0.13
(2,1255)	1:52:A:LEU:HD11	1:54:A:SER:H	1	0.13
(2,1200)	1:43:A:GLU:HG3	1:41:A:TYR:H	7	0.13
(2,1200)	1:43:A:GLU:HG3	1:41:A:TYR:H	17	0.13
(2,1179)	1:18:A:PRO:HD3	1:20:A:GLU:H	12	0.13
(2,1179)	1:35:A:ARG:HD3	1:20:A:GLU:H	18	0.13
(2,1179)	1:35:A:ARG:HD3	1:20:A:GLU:H	19	0.13
(2,1166)	1:124:A:SER:HB3	1:124:A:SER:H	14	0.13
(2,1109)	1:97:A:ARG:H	1:95:A:LEU:H	1	0.13
(2,1104)	1:36:A:LEU:H	1:20:A:GLU:H	16	0.13
(2,1017)	1:45:A:LYS:HD2	1:117:A:SER:H	18	0.13
(2,962)	1:95:A:LEU:HA	1:97:A:ARG:H	4	0.13
(2,895)	1:91:A:ILE:HD12	1:88:A:LYS:H	6	0.13
(2,886)	1:28:A:LEU:HD12	1:26:A:ASP:H	10	0.13
(2,885)	1:66:A:ILE:HD13	1:26:A:ASP:H	4	0.13
(2,871)	1:119:A:ILE:HD13	1:119:A:ILE:H	7	0.13
(2,862)	1:111:A:LEU:HD23	1:111:A:LEU:H	1	0.13
(2,862)	1:111:A:LEU:HD21	1:111:A:LEU:H	20	0.13
(2,848)	1:27:A:ALA:HB2	1:26:A:ASP:H	4	0.13
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	6	0.13
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	6	0.13
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	6	0.13
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	20	0.13
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	20	0.13
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	20	0.13
(2,844)	1:94:A:LEU:HD21	1:94:A:LEU:H	4	0.13
(2,841)	1:5:A:ILE:HD12	1:5:A:ILE:H	1	0.13
(2,831)	1:119:A:ILE:HD11	1:112:A:LEU:H	2	0.13
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	18	0.13
(2,816)	1:51:A:LYS:HG2	1:49:A:VAL:H	4	0.13
(2,791)	1:111:A:LEU:HB3	1:112:A:LEU:H	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,784)	1:61:A:TRP:HB2	1:24:A:ILE:H	9	0.13
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	6	0.13
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	15	0.13
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	17	0.13
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	19	0.13
(2,764)	1:46:A:LYS:HE2	1:28:A:LEU:H	13	0.13
(2,708)	1:84:A:GLU:HA	1:87:A:ASN:H	11	0.13
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	2	0.13
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	3	0.13
(2,677)	1:78:A:GLU:HA	1:103:A:ILE:H	11	0.13
(2,571)	1:118:A:LEU:HD13	1:52:A:LEU:H	6	0.13
(2,565)	1:102:A:VAL:HG13	1:79:A:TYR:H	2	0.13
(2,560)	1:95:A:LEU:HD11	1:104:A:LEU:H	4	0.13
(2,558)	1:104:A:LEU:HD21	1:104:A:LEU:H	3	0.13
(2,558)	1:104:A:LEU:HD22	1:104:A:LEU:H	3	0.13
(2,558)	1:104:A:LEU:HD23	1:104:A:LEU:H	3	0.13
(2,554)	1:71:A:ILE:HG23	1:80:A:PHE:H	18	0.13
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	2	0.13
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	14	0.13
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	18	0.13
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	4	0.13
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	7	0.13
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	15	0.13
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	6	0.13
(2,293)	1:129:A:TYR:HA	1:129:A:TYR:H	5	0.13
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	1	0.13
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	6	0.13
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	10	0.13
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	13	0.13
(2,260)	1:94:A:LEU:HD12	1:93:A:ILE:H	20	0.13
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	9	0.13
(2,253)	1:22:A:VAL:HG22	1:27:A:ALA:H	4	0.13
(2,225)	1:98:A:GLU:HG2	1:99:A:ILE:H	5	0.13
(2,156)	1:69:A:ILE:HD11	1:120:A:PHE:H	3	0.13
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	11	0.13
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	6	0.13
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	10	0.13
(2,123)	1:28:A:LEU:HA	1:31:A:LYS:H	14	0.13
(2,100)	1:79:A:TYR:HE2	1:70:A:PHE:H	17	0.13
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	1	0.13
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	3	0.13
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4669)	1:69:A:ILE:HG12	1:21:A:TYR:HE1	18	0.12
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE2	3	0.12
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE1	6	0.12
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE1	8	0.12
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE1	9	0.12
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE1	14	0.12
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE2	15	0.12
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE1	9	0.12
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE2	10	0.12
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE1	11	0.12
(2,4658)	1:79:A:TYR:HB3	1:79:A:TYR:HE2	16	0.12
(2,4648)	1:20:A:GLU:HA	1:21:A:TYR:HE2	18	0.12
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE1	19	0.12
(2,4641)	1:78:A:GLU:HA	1:79:A:TYR:HE1	17	0.12
(2,4474)	1:36:A:LEU:HD21	1:41:A:TYR:HD1	2	0.12
(2,4474)	1:36:A:LEU:HD23	1:41:A:TYR:HD2	17	0.12
(2,4469)	1:69:A:ILE:HD13	1:21:A:TYR:HD1	16	0.12
(2,4465)	1:118:A:LEU:HD11	1:115:A:TYR:HD1	4	0.12
(2,4459)	1:33:A:LYS:HB3	1:41:A:TYR:HD2	9	0.12
(2,4438)	1:35:A:ARG:HD3	1:41:A:TYR:HD2	14	0.12
(2,4333)	1:18:A:PRO:HD3	1:69:A:ILE:HD12	20	0.12
(2,4324)	1:91:A:ILE:H	1:56:A:ILE:HD11	5	0.12
(2,4324)	1:91:A:ILE:H	1:56:A:ILE:HD13	9	0.12
(2,4320)	1:24:A:ILE:HB	1:66:A:ILE:HG23	3	0.12
(2,4320)	1:24:A:ILE:HB	1:66:A:ILE:HG23	13	0.12
(2,4279)	1:68:A:PHE:HD1	1:118:A:LEU:HD11	16	0.12
(2,4264)	1:101:A:ASN:HB2	1:102:A:VAL:HB	20	0.12
(2,4207)	1:70:A:PHE:HE2	1:91:A:ILE:HD11	13	0.12
(2,4203)	1:95:A:LEU:H	1:91:A:ILE:HD12	9	0.12
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD12	5	0.12
(2,4057)	1:122:A:ILE:H	1:121:A:ILE:HD12	9	0.12
(2,4025)	1:111:A:LEU:HB3	1:119:A:ILE:HG21	1	0.12
(2,4020)	1:49:A:VAL:HB	1:44:A:ILE:HG22	11	0.12
(2,4012)	1:68:A:PHE:HB3	1:66:A:ILE:HG21	10	0.12
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG23	5	0.12
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG21	4	0.12
(2,3911)	1:70:A:PHE:HE2	1:103:A:ILE:HG21	13	0.12
(2,3896)	1:115:A:TYR:H	1:119:A:ILE:HG23	11	0.12
(2,3866)	1:23:A:THR:H	1:27:A:ALA:HB2	6	0.12
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG12	8	0.12
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG11	11	0.12
(2,3809)	1:88:A:LYS:HD3	1:81:A:VAL:HG11	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG11	12	0.12
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG12	12	0.12
(2,3795)	1:88:A:LYS:HE2	1:81:A:VAL:HG13	12	0.12
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG23	11	0.12
(2,3681)	1:75:A:GLU:H	1:126:A:THR:HG22	13	0.12
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG11	17	0.12
(2,3664)	1:103:A:ILE:H	1:81:A:VAL:HG11	1	0.12
(2,3632)	1:94:A:LEU:HD12	1:95:A:LEU:HG	18	0.12
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	4	0.12
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	5	0.12
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	8	0.12
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	11	0.12
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	12	0.12
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	14	0.12
(2,3614)	1:60:A:LEU:HB2	1:64:A:VAL:HG22	14	0.12
(2,3471)	1:118:A:LEU:HA	1:44:A:ILE:HG12	7	0.12
(2,3467)	1:51:A:LYS:HA	1:51:A:LYS:HG2	1	0.12
(2,3445)	1:56:A:ILE:HA	1:52:A:LEU:HD11	15	0.12
(2,3439)	1:42:A:HIS:HA	1:36:A:LEU:HD12	2	0.12
(2,3405)	1:115:A:TYR:HE2	1:118:A:LEU:HD12	13	0.12
(2,3405)	1:115:A:TYR:HE2	1:118:A:LEU:HD12	14	0.12
(2,3389)	1:41:A:TYR:HD1	1:36:A:LEU:HG	3	0.12
(2,3389)	1:41:A:TYR:HD2	1:36:A:LEU:HG	9	0.12
(2,3281)	1:72:A:LYS:H	1:71:A:ILE:HG13	19	0.12
(2,3265)	1:94:A:LEU:HD12	1:91:A:ILE:HG12	16	0.12
(2,3265)	1:94:A:LEU:HD12	1:91:A:ILE:HG12	20	0.12
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	16	0.12
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	4	0.12
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	5	0.12
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	8	0.12
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	11	0.12
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	12	0.12
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	14	0.12
(2,2955)	1:75:A:GLU:HA	1:75:A:GLU:HG3	14	0.12
(2,2865)	1:104:A:LEU:HD23	1:105:A:ASN:HB3	1	0.12
(2,2845)	1:51:A:LYS:HG2	1:47:A:ASP:HB2	10	0.12
(2,2844)	1:51:A:LYS:HG2	1:47:A:ASP:HB3	6	0.12
(2,2827)	1:45:A:LYS:HB3	1:47:A:ASP:HB3	13	0.12
(2,2827)	1:50:A:GLU:HB2	1:47:A:ASP:HB3	14	0.12
(2,2819)	1:81:A:VAL:HB	1:101:A:ASN:HB2	5	0.12
(2,2819)	1:81:A:VAL:HB	1:101:A:ASN:HB2	10	0.12
(2,2634)	1:35:A:ARG:HB3	1:35:A:ARG:HD3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	7	0.12
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	12	0.12
(2,2538)	1:115:A:TYR:HD1	1:118:A:LEU:HB3	15	0.12
(2,2473)	1:69:A:ILE:HD12	1:18:A:PRO:HD3	20	0.12
(2,2372)	1:34:A:ILE:HG21	1:21:A:TYR:HA	20	0.12
(2,2356)	1:19:A:ALA:HB1	1:36:A:LEU:HA	10	0.12
(2,2356)	1:19:A:ALA:HB3	1:36:A:LEU:HA	15	0.12
(2,2318)	1:50:A:GLU:HB2	1:47:A:ASP:HA	1	0.12
(2,2179)	1:108:A:VAL:HG12	1:105:A:ASN:HA	15	0.12
(2,2173)	1:118:A:LEU:HD12	1:48:A:GLU:HA	8	0.12
(2,2143)	1:133:A:THR:HG21	1:134:A:GLU:HA	16	0.12
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	10	0.12
(2,2051)	1:80:A:PHE:HB2	1:102:A:VAL:HA	4	0.12
(2,1946)	1:27:A:ALA:H	1:22:A:VAL:HA	12	0.12
(2,1870)	1:8:A:ILE:HG12	1:8:A:ILE:HA	10	0.12
(2,1847)	1:78:A:GLU:HB3	1:73:A:SER:HB2	15	0.12
(2,1828)	1:125:A:PRO:HB2	1:125:A:PRO:HA	19	0.12
(2,1819)	1:105:A:ASN:HB2	1:106:A:VAL:HA	11	0.12
(2,1781)	1:68:A:PHE:HE2	1:91:A:ILE:HA	1	0.12
(2,1731)	1:56:A:ILE:HG21	1:24:A:ILE:HA	10	0.12
(2,1729)	1:52:A:LEU:HG	1:49:A:VAL:HA	19	0.12
(2,1718)	1:64:A:VAL:HB	1:24:A:ILE:HA	7	0.12
(2,1677)	1:65:A:LYS:HE3	1:23:A:THR:HB	8	0.12
(2,1632)	1:138:A:MET:HB3	1:136:A:SER:H	18	0.12
(2,1627)	1:135:A:LEU:HD11	1:133:A:THR:H	3	0.12
(2,1627)	1:135:A:LEU:HD12	1:133:A:THR:H	3	0.12
(2,1627)	1:135:A:LEU:HD13	1:133:A:THR:H	3	0.12
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	1	0.12
(2,1611)	1:86:A:TRP:HD1	1:84:A:GLU:H	17	0.12
(2,1599)	1:141:A:HIS:HA	1:140:A:GLU:H	10	0.12
(2,1595)	1:95:A:LEU:HD13	1:107:A:ASP:H	12	0.12
(2,1541)	1:22:A:VAL:HB	1:30:A:GLY:H	5	0.12
(2,1540)	1:46:A:LYS:HB2	1:30:A:GLY:H	14	0.12
(2,1523)	1:63:A:LEU:HG	1:62:A:SER:H	7	0.12
(2,1523)	1:63:A:LEU:HG	1:62:A:SER:H	14	0.12
(2,1523)	1:63:A:LEU:HG	1:62:A:SER:H	19	0.12
(2,1389)	1:106:A:VAL:HG23	1:105:A:ASN:HD21	5	0.12
(2,1386)	1:65:A:LYS:HD3	1:21:A:TYR:H	1	0.12
(2,1378)	1:109:A:GLU:HB2	1:105:A:ASN:HD22	2	0.12
(2,1350)	1:50:A:GLU:HB3	1:53:A:SER:H	13	0.12
(2,1253)	1:52:A:LEU:HD11	1:56:A:ILE:H	2	0.12
(2,1244)	1:34:A:ILE:HD11	1:20:A:GLU:H	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1229)	1:130:A:THR:HG21	1:130:A:THR:H	20	0.12
(2,1229)	1:130:A:THR:HG22	1:130:A:THR:H	20	0.12
(2,1229)	1:130:A:THR:HG23	1:130:A:THR:H	20	0.12
(2,1220)	1:99:A:ILE:HG13	1:101:A:ASN:H	6	0.12
(2,1200)	1:43:A:GLU:HG3	1:41:A:TYR:H	4	0.12
(2,1196)	1:45:A:LYS:HB2	1:47:A:ASP:H	4	0.12
(2,1191)	1:132:A:GLU:HG2	1:133:A:THR:H	19	0.12
(2,1188)	1:37:A:ASN:HB2	1:15:A:SER:H	3	0.12
(2,1188)	1:37:A:ASN:HB2	1:15:A:SER:H	9	0.12
(2,1180)	1:45:A:LYS:HE2	1:47:A:ASP:H	7	0.12
(2,1150)	1:111:A:LEU:HA	1:113:A:ARG:H	12	0.12
(2,1025)	1:118:A:LEU:HB2	1:115:A:TYR:H	9	0.12
(2,1011)	1:61:A:TRP:HB2	1:25:A:LYS:H	8	0.12
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	1	0.12
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	16	0.12
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	19	0.12
(2,886)	1:24:A:ILE:HG23	1:26:A:ASP:H	12	0.12
(2,877)	1:60:A:LEU:HD22	1:86:A:TRP:H	16	0.12
(2,871)	1:119:A:ILE:HD11	1:119:A:ILE:H	5	0.12
(2,855)	1:64:A:VAL:HG13	1:87:A:ASN:H	15	0.12
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	7	0.12
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	7	0.12
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	7	0.12
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	8	0.12
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	8	0.12
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	8	0.12
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	12	0.12
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	12	0.12
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	12	0.12
(2,844)	1:94:A:LEU:HD23	1:94:A:LEU:H	3	0.12
(2,841)	1:5:A:ILE:HD13	1:5:A:ILE:H	15	0.12
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	4	0.12
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	12	0.12
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	16	0.12
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	18	0.12
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	20	0.12
(2,764)	1:29:A:ASP:HB3	1:28:A:LEU:H	20	0.12
(2,760)	1:33:A:LYS:HE3	1:34:A:ILE:H	15	0.12
(2,744)	1:86:A:TRP:HB2	1:87:A:ASN:H	13	0.12
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	18	0.12
(2,605)	1:28:A:LEU:HD22	1:51:A:LYS:H	10	0.12
(2,573)	1:71:A:ILE:HG12	1:69:A:ILE:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,568)	1:49:A:VAL:HG11	1:50:A:GLU:H	18	0.12
(2,568)	1:49:A:VAL:HG12	1:50:A:GLU:H	18	0.12
(2,568)	1:49:A:VAL:HG13	1:50:A:GLU:H	18	0.12
(2,558)	1:104:A:LEU:HD21	1:104:A:LEU:H	10	0.12
(2,558)	1:104:A:LEU:HD22	1:104:A:LEU:H	10	0.12
(2,558)	1:104:A:LEU:HD23	1:104:A:LEU:H	10	0.12
(2,552)	1:104:A:LEU:HB3	1:107:A:ASP:H	19	0.12
(2,527)	1:72:A:LYS:HB2	1:79:A:TYR:H	2	0.12
(2,516)	1:72:A:LYS:HD2	1:80:A:PHE:H	8	0.12
(2,516)	1:72:A:LYS:HB2	1:80:A:PHE:H	16	0.12
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	2	0.12
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	6	0.12
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	12	0.12
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	17	0.12
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	19	0.12
(2,426)	1:18:A:PRO:HA	1:42:A:HIS:H	15	0.12
(2,334)	1:60:A:LEU:HG	1:61:A:TRP:H	4	0.12
(2,312)	1:131:A:GLU:HG2	1:131:A:GLU:H	9	0.12
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	11	0.12
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	12	0.12
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	14	0.12
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	2	0.12
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	11	0.12
(2,161)	1:69:A:ILE:HG21	1:70:A:PHE:H	18	0.12
(2,158)	1:122:A:ILE:HG23	1:123:A:LEU:H	19	0.12
(2,154)	1:71:A:ILE:HD13	1:122:A:ILE:H	18	0.12
(2,144)	1:121:A:ILE:HB	1:70:A:PHE:H	4	0.12
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	3	0.12
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	4	0.12
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	16	0.12
(2,118)	1:124:A:SER:HB2	1:123:A:LEU:H	12	0.12
(2,95)	1:70:A:PHE:HD1	1:122:A:ILE:H	10	0.12
(2,84)	1:24:A:ILE:HG23	1:61:A:TRP:HE1	10	0.12
(2,80)	1:34:A:ILE:HG21	1:35:A:ARG:H	10	0.12
(2,34)	1:71:A:ILE:HG22	1:72:A:LYS:H	6	0.12
(2,33)	1:46:A:LYS:HD3	1:46:A:LYS:H	12	0.12
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE1	18	0.11
(2,4701)	1:128:A:SER:HB3	1:129:A:TYR:HE2	18	0.11
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE2	7	0.11
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE2	13	0.11
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE1	17	0.11
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE2	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4647)	1:68:A:PHE:HA	1:21:A:TYR:HE2	12	0.11
(2,4536)	1:70:A:PHE:HB2	1:70:A:PHE:HE1	20	0.11
(2,4512)	1:121:A:ILE:HD13	1:79:A:TYR:HD1	18	0.11
(2,4506)	1:13:A:ILE:HG12	1:14:A:PHE:HD1	9	0.11
(2,4506)	1:13:A:ILE:HG12	1:14:A:PHE:HD2	9	0.11
(2,4474)	1:36:A:LEU:HD23	1:41:A:TYR:HD2	5	0.11
(2,4465)	1:118:A:LEU:HD11	1:115:A:TYR:HD1	10	0.11
(2,4460)	1:72:A:LYS:HB3	1:79:A:TYR:HD2	16	0.11
(2,4459)	1:33:A:LYS:HB3	1:41:A:TYR:HD1	6	0.11
(2,4401)	1:119:A:ILE:H	1:116:A:THR:HB	17	0.11
(2,4398)	1:52:A:LEU:HA	1:55:A:ARG:HD2	10	0.11
(2,4324)	1:91:A:ILE:H	1:56:A:ILE:HD11	4	0.11
(2,4320)	1:24:A:ILE:HB	1:66:A:ILE:HG22	11	0.11
(2,4266)	1:5:A:ILE:HG12	1:4:A:LYS:HB2	12	0.11
(2,4266)	1:5:A:ILE:HG12	1:4:A:LYS:HB3	12	0.11
(2,4243)	1:102:A:VAL:HG22	1:104:A:LEU:HA	9	0.11
(2,4207)	1:70:A:PHE:HE1	1:91:A:ILE:HD12	1	0.11
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD12	4	0.11
(2,4158)	1:115:A:TYR:HB3	1:119:A:ILE:HD12	10	0.11
(2,4100)	1:61:A:TRP:HZ3	1:24:A:ILE:HG21	19	0.11
(2,4080)	1:28:A:LEU:H	1:24:A:ILE:HG23	15	0.11
(2,4012)	1:68:A:PHE:HB3	1:66:A:ILE:HG23	16	0.11
(2,3972)	1:68:A:PHE:HA	1:66:A:ILE:HG21	18	0.11
(2,3961)	1:32:A:LEU:HA	1:22:A:VAL:HG23	3	0.11
(2,3919)	1:39:A:ASN:HD22	1:19:A:ALA:HB2	14	0.11
(2,3911)	1:70:A:PHE:HE2	1:103:A:ILE:HG21	11	0.11
(2,3908)	1:48:A:GLU:H	1:44:A:ILE:HG21	10	0.11
(2,3908)	1:48:A:GLU:H	1:44:A:ILE:HG22	12	0.11
(2,3900)	1:64:A:VAL:H	1:90:A:ALA:HB3	19	0.11
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG21	6	0.11
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG22	6	0.11
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG23	6	0.11
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG21	6	0.11
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG22	6	0.11
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG23	6	0.11
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG21	6	0.11
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG22	6	0.11
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG23	6	0.11
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG21	15	0.11
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG22	15	0.11
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG23	15	0.11
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG21	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG22	15	0.11
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG23	15	0.11
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG21	15	0.11
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG22	15	0.11
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG23	15	0.11
(2,3803)	1:42:A:HIS:HB2	1:36:A:LEU:HD23	12	0.11
(2,3784)	1:28:A:LEU:HA	1:32:A:LEU:HD21	18	0.11
(2,3756)	1:116:A:THR:HA	1:112:A:LEU:HD22	13	0.11
(2,3714)	1:49:A:VAL:H	1:28:A:LEU:HD23	17	0.11
(2,3708)	1:33:A:LYS:H	1:22:A:VAL:HG11	5	0.11
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG11	4	0.11
(2,3672)	1:103:A:ILE:H	1:102:A:VAL:HG11	14	0.11
(2,3670)	1:79:A:TYR:H	1:104:A:LEU:HD23	18	0.11
(2,3624)	1:56:A:ILE:HG21	1:94:A:LEU:HD13	20	0.11
(2,3618)	1:57:A:PRO:HB2	1:60:A:LEU:HG	1	0.11
(2,3614)	1:60:A:LEU:HB2	1:64:A:VAL:HG22	12	0.11
(2,3601)	1:56:A:ILE:HB	1:52:A:LEU:HD13	18	0.11
(2,3434)	1:33:A:LYS:HA	1:34:A:ILE:HG12	17	0.11
(2,3361)	1:87:A:ASN:HD22	1:64:A:VAL:HG23	3	0.11
(2,3354)	1:61:A:TRP:HZ3	1:25:A:LYS:HG3	12	0.11
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	3	0.11
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	16	0.11
(2,3281)	1:72:A:LYS:H	1:71:A:ILE:HG13	2	0.11
(2,3265)	1:94:A:LEU:HD11	1:91:A:ILE:HG12	2	0.11
(2,3256)	1:95:A:LEU:HD21	1:110:A:LYS:HD2	2	0.11
(2,3256)	1:95:A:LEU:HD21	1:110:A:LYS:HD3	2	0.11
(2,3256)	1:95:A:LEU:HD22	1:110:A:LYS:HD2	2	0.11
(2,3256)	1:95:A:LEU:HD22	1:110:A:LYS:HD3	2	0.11
(2,3256)	1:95:A:LEU:HD23	1:110:A:LYS:HD2	2	0.11
(2,3256)	1:95:A:LEU:HD23	1:110:A:LYS:HD3	2	0.11
(2,3246)	1:135:A:LEU:HD12	1:138:A:MET:HG2	9	0.11
(2,3011)	1:60:A:LEU:HG	1:57:A:PRO:HB2	1	0.11
(2,2961)	1:52:A:LEU:HA	1:114:A:GLU:HG2	4	0.11
(2,2960)	1:52:A:LEU:HA	1:114:A:GLU:HG3	18	0.11
(2,2865)	1:76:A:ILE:HG22	1:105:A:ASN:HB2	16	0.11
(2,2865)	1:104:A:LEU:HD23	1:105:A:ASN:HB3	20	0.11
(2,2827)	1:50:A:GLU:HB2	1:47:A:ASP:HB3	9	0.11
(2,2822)	1:118:A:LEU:HB3	1:115:A:TYR:HB2	19	0.11
(2,2817)	1:36:A:LEU:HB3	1:40:A:PHE:HB3	9	0.11
(2,2569)	1:79:A:TYR:HA	1:80:A:PHE:HB3	19	0.11
(2,2560)	1:42:A:HIS:HD2	1:34:A:ILE:HB	5	0.11
(2,2340)	1:114:A:GLU:HB3	1:115:A:TYR:HA	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2340)	1:114:A:GLU:HB3	1:115:A:TYR:HA	20	0.11
(2,2318)	1:110:A:LYS:HB2	1:107:A:ASP:HA	5	0.11
(2,2318)	1:50:A:GLU:HB2	1:47:A:ASP:HA	7	0.11
(2,2318)	1:50:A:GLU:HB2	1:47:A:ASP:HA	15	0.11
(2,2179)	1:108:A:VAL:HG13	1:105:A:ASN:HA	9	0.11
(2,2179)	1:108:A:VAL:HG12	1:105:A:ASN:HA	19	0.11
(2,2173)	1:118:A:LEU:HD12	1:48:A:GLU:HA	12	0.11
(2,2123)	1:65:A:LYS:HG2	1:22:A:VAL:HA	14	0.11
(2,1903)	1:122:A:ILE:HD11	1:17:A:SER:HB2	15	0.11
(2,1903)	1:122:A:ILE:HD11	1:17:A:SER:HB3	15	0.11
(2,1903)	1:122:A:ILE:HD12	1:17:A:SER:HB2	15	0.11
(2,1903)	1:122:A:ILE:HD12	1:17:A:SER:HB3	15	0.11
(2,1903)	1:122:A:ILE:HD13	1:17:A:SER:HB2	15	0.11
(2,1903)	1:122:A:ILE:HD13	1:17:A:SER:HB3	15	0.11
(2,1781)	1:68:A:PHE:HE2	1:91:A:ILE:HA	9	0.11
(2,1734)	1:112:A:LEU:HD22	1:116:A:THR:HA	13	0.11
(2,1717)	1:49:A:VAL:HB	1:24:A:ILE:HA	7	0.11
(2,1654)	1:41:A:TYR:HB3	1:36:A:LEU:H	15	0.11
(2,1629)	1:77:A:GLY:HA2	1:105:A:ASN:HD21	16	0.11
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	5	0.11
(2,1625)	1:47:A:ASP:HB3	1:47:A:ASP:H	9	0.11
(2,1617)	1:111:A:LEU:HB3	1:115:A:TYR:H	4	0.11
(2,1617)	1:111:A:LEU:HB3	1:115:A:TYR:H	9	0.11
(2,1611)	1:86:A:TRP:HD1	1:84:A:GLU:H	3	0.11
(2,1599)	1:62:A:SER:HA	1:26:A:ASP:H	8	0.11
(2,1599)	1:62:A:SER:HA	1:26:A:ASP:H	11	0.11
(2,1566)	1:79:A:TYR:HA	1:81:A:VAL:H	20	0.11
(2,1523)	1:63:A:LEU:HG	1:62:A:SER:H	3	0.11
(2,1523)	1:63:A:LEU:HG	1:62:A:SER:H	6	0.11
(2,1499)	1:93:A:ILE:HG22	1:96:A:GLY:H	6	0.11
(2,1390)	1:99:A:ILE:HG21	1:101:A:ASN:HD21	7	0.11
(2,1390)	1:99:A:ILE:HG22	1:101:A:ASN:HD21	7	0.11
(2,1390)	1:99:A:ILE:HG23	1:101:A:ASN:HD21	7	0.11
(2,1350)	1:50:A:GLU:HB3	1:53:A:SER:H	20	0.11
(2,1330)	1:137:A:GLU:HG2	1:136:A:SER:H	8	0.11
(2,1273)	1:115:A:TYR:HD1	1:53:A:SER:H	2	0.11
(2,1273)	1:115:A:TYR:HD2	1:53:A:SER:H	16	0.11
(2,1244)	1:34:A:ILE:HD11	1:20:A:GLU:H	1	0.11
(2,1229)	1:130:A:THR:HG21	1:130:A:THR:H	5	0.11
(2,1229)	1:130:A:THR:HG22	1:130:A:THR:H	5	0.11
(2,1229)	1:130:A:THR:HG23	1:130:A:THR:H	5	0.11
(2,1229)	1:130:A:THR:HG21	1:130:A:THR:H	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1229)	1:130:A:THR:HG22	1:130:A:THR:H	14	0.11
(2,1229)	1:130:A:THR:HG23	1:130:A:THR:H	14	0.11
(2,1205)	1:123:A:LEU:HB3	1:124:A:SER:H	9	0.11
(2,1199)	1:102:A:VAL:HB	1:101:A:ASN:H	4	0.11
(2,1196)	1:45:A:LYS:HB2	1:47:A:ASP:H	8	0.11
(2,1193)	1:37:A:ASN:HB3	1:38:A:ASN:H	16	0.11
(2,1188)	1:37:A:ASN:HB2	1:15:A:SER:H	13	0.11
(2,1055)	1:99:A:ILE:HG12	1:92:A:SER:H	2	0.11
(2,1030)	1:22:A:VAL:HB	1:29:A:ASP:H	2	0.11
(2,1030)	1:22:A:VAL:HB	1:29:A:ASP:H	19	0.11
(2,1025)	1:118:A:LEU:HB2	1:115:A:TYR:H	7	0.11
(2,980)	1:141:A:HIS:HB2	1:141:A:HIS:H	1	0.11
(2,974)	1:87:A:ASN:HB3	1:84:A:GLU:H	11	0.11
(2,932)	1:68:A:PHE:HZ	1:91:A:ILE:H	5	0.11
(2,910)	1:31:A:LYS:H	1:29:A:ASP:H	7	0.11
(2,871)	1:119:A:ILE:HD11	1:119:A:ILE:H	10	0.11
(2,862)	1:111:A:LEU:HD21	1:111:A:LEU:H	17	0.11
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	3	0.11
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	3	0.11
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	3	0.11
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	4	0.11
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	4	0.11
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	4	0.11
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	9	0.11
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	9	0.11
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	9	0.11
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	18	0.11
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	18	0.11
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	18	0.11
(2,844)	1:94:A:LEU:HD21	1:94:A:LEU:H	7	0.11
(2,833)	1:33:A:LYS:HG2	1:34:A:ILE:H	16	0.11
(2,831)	1:119:A:ILE:HD12	1:112:A:LEU:H	6	0.11
(2,828)	1:45:A:LYS:HB2	1:48:A:GLU:H	9	0.11
(2,819)	1:110:A:LYS:HD3	1:111:A:LEU:H	15	0.11
(2,816)	1:51:A:LYS:HG2	1:49:A:VAL:H	10	0.11
(2,808)	1:11:A:LYS:HD2	1:12:A:ASP:H	7	0.11
(2,808)	1:11:A:LYS:HD3	1:12:A:ASP:H	7	0.11
(2,791)	1:111:A:LEU:HB3	1:112:A:LEU:H	16	0.11
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	3	0.11
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	8	0.11
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	11	0.11
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,708)	1:84:A:GLU:HA	1:87:A:ASN:H	13	0.11
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	10	0.11
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	14	0.11
(2,685)	1:110:A:LYS:HA	1:112:A:LEU:H	15	0.11
(2,677)	1:78:A:GLU:HA	1:103:A:ILE:H	12	0.11
(2,582)	1:56:A:ILE:HG13	1:55:A:ARG:H	14	0.11
(2,571)	1:118:A:LEU:HD11	1:52:A:LEU:H	3	0.11
(2,568)	1:49:A:VAL:HG11	1:50:A:GLU:H	13	0.11
(2,568)	1:49:A:VAL:HG12	1:50:A:GLU:H	13	0.11
(2,568)	1:49:A:VAL:HG13	1:50:A:GLU:H	13	0.11
(2,568)	1:49:A:VAL:HG11	1:50:A:GLU:H	16	0.11
(2,568)	1:49:A:VAL:HG12	1:50:A:GLU:H	16	0.11
(2,568)	1:49:A:VAL:HG13	1:50:A:GLU:H	16	0.11
(2,568)	1:49:A:VAL:HG11	1:50:A:GLU:H	20	0.11
(2,568)	1:49:A:VAL:HG12	1:50:A:GLU:H	20	0.11
(2,568)	1:49:A:VAL:HG13	1:50:A:GLU:H	20	0.11
(2,564)	1:104:A:LEU:HD23	1:79:A:TYR:H	18	0.11
(2,558)	1:104:A:LEU:HD21	1:104:A:LEU:H	2	0.11
(2,558)	1:104:A:LEU:HD22	1:104:A:LEU:H	2	0.11
(2,558)	1:104:A:LEU:HD23	1:104:A:LEU:H	2	0.11
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	3	0.11
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	5	0.11
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	13	0.11
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	18	0.11
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	20	0.11
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	4	0.11
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	16	0.11
(2,294)	1:127:A:ARG:HA	1:127:A:ARG:H	1	0.11
(2,293)	1:129:A:TYR:HA	1:129:A:TYR:H	4	0.11
(2,293)	1:129:A:TYR:HA	1:129:A:TYR:H	7	0.11
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	7	0.11
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	8	0.11
(2,291)	1:75:A:GLU:HA	1:75:A:GLU:H	15	0.11
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	8	0.11
(2,205)	1:90:A:ALA:HA	1:93:A:ILE:H	4	0.11
(2,205)	1:90:A:ALA:HA	1:93:A:ILE:H	10	0.11
(2,205)	1:90:A:ALA:HA	1:93:A:ILE:H	16	0.11
(2,160)	1:121:A:ILE:HG21	1:70:A:PHE:H	19	0.11
(2,156)	1:69:A:ILE:HD11	1:120:A:PHE:H	11	0.11
(2,154)	1:71:A:ILE:HD13	1:122:A:ILE:H	5	0.11
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	1	0.11
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	19	0.11
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	20	0.11
(2,123)	1:28:A:LEU:HA	1:31:A:LYS:H	18	0.11
(2,95)	1:70:A:PHE:HD2	1:122:A:ILE:H	4	0.11
(2,84)	1:24:A:ILE:HG21	1:61:A:TRP:HE1	14	0.11
(2,84)	1:24:A:ILE:HG23	1:61:A:TRP:HE1	20	0.11
(2,27)	1:45:A:LYS:HE2	1:46:A:LYS:H	15	0.11
(2,27)	1:45:A:LYS:HE3	1:46:A:LYS:H	15	0.11
(2,27)	1:45:A:LYS:HE2	1:46:A:LYS:H	19	0.11
(2,27)	1:45:A:LYS:HE3	1:46:A:LYS:H	19	0.11
(2,9)	1:85:A:GLN:HB3	1:86:A:TRP:HE1	8	0.11
(2,4660)	1:41:A:TYR:HB2	1:41:A:TYR:HE2	1	0.1
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE2	5	0.1
(2,4660)	1:21:A:TYR:HB2	1:21:A:TYR:HE1	11	0.1
(2,4536)	1:70:A:PHE:HB2	1:70:A:PHE:HE2	9	0.1
(2,4536)	1:70:A:PHE:HB2	1:70:A:PHE:HE1	14	0.1
(2,4465)	1:118:A:LEU:HD12	1:115:A:TYR:HD1	6	0.1
(2,4279)	1:68:A:PHE:HD2	1:118:A:LEU:HD11	12	0.1
(2,4168)	1:57:A:PRO:HB3	1:93:A:ILE:HD12	8	0.1
(2,4068)	1:103:A:ILE:H	1:103:A:ILE:HD11	11	0.1
(2,4066)	1:45:A:LYS:H	1:66:A:ILE:HD13	20	0.1
(2,4011)	1:68:A:PHE:HB3	1:119:A:ILE:HG21	3	0.1
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG21	10	0.1
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG22	10	0.1
(2,3847)	1:112:A:LEU:HD21	1:116:A:THR:HG23	10	0.1
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG21	10	0.1
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG22	10	0.1
(2,3847)	1:112:A:LEU:HD22	1:116:A:THR:HG23	10	0.1
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG21	10	0.1
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG22	10	0.1
(2,3847)	1:112:A:LEU:HD23	1:116:A:THR:HG23	10	0.1
(2,3811)	1:48:A:GLU:HB2	1:49:A:VAL:HG23	9	0.1
(2,3805)	1:86:A:TRP:HB2	1:63:A:LEU:HD11	8	0.1
(2,3805)	1:86:A:TRP:HB2	1:63:A:LEU:HD12	8	0.1
(2,3805)	1:86:A:TRP:HB2	1:63:A:LEU:HD13	8	0.1
(2,3793)	1:72:A:LYS:HA	1:108:A:VAL:HG22	3	0.1
(2,3784)	1:28:A:LEU:HA	1:32:A:LEU:HD23	13	0.1
(2,3714)	1:49:A:VAL:H	1:28:A:LEU:HD21	4	0.1
(2,3632)	1:94:A:LEU:HD12	1:95:A:LEU:HG	6	0.1
(2,3632)	1:94:A:LEU:HD12	1:95:A:LEU:HG	7	0.1
(2,3614)	1:60:A:LEU:HB2	1:64:A:VAL:HG21	5	0.1
(2,3389)	1:41:A:TYR:HD1	1:36:A:LEU:HG	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3389)	1:41:A:TYR:HD1	1:36:A:LEU:HG	19	0.1
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	2	0.1
(2,3346)	1:20:A:GLU:H	1:18:A:PRO:HG3	13	0.1
(2,3201)	1:51:A:LYS:HE3	1:114:A:GLU:HB2	5	0.1
(2,3072)	1:86:A:TRP:HH2	1:85:A:GLN:HG2	13	0.1
(2,2991)	1:93:A:ILE:HG23	1:57:A:PRO:HB3	20	0.1
(2,2963)	1:68:A:PHE:HA	1:67:A:PRO:HB2	2	0.1
(2,2825)	1:31:A:LYS:HB3	1:26:A:ASP:HB2	12	0.1
(2,2490)	1:31:A:LYS:HG2	1:30:A:GLY:HA3	20	0.1
(2,2466)	1:69:A:ILE:HG23	1:70:A:PHE:HA	12	0.1
(2,2356)	1:19:A:ALA:HB2	1:36:A:LEU:HA	7	0.1
(2,2340)	1:114:A:GLU:HB3	1:115:A:TYR:HA	17	0.1
(2,2179)	1:108:A:VAL:HG13	1:105:A:ASN:HA	14	0.1
(2,2143)	1:133:A:THR:HG22	1:134:A:GLU:HA	19	0.1
(2,1998)	1:115:A:TYR:HD1	1:112:A:LEU:HA	5	0.1
(2,1990)	1:14:A:PHE:HD2	1:11:A:LYS:HA	11	0.1
(2,1948)	1:92:A:SER:H	1:99:A:ILE:HA	6	0.1
(2,1877)	1:137:A:GLU:HB2	1:136:A:SER:HB2	12	0.1
(2,1870)	1:8:A:ILE:HG12	1:8:A:ILE:HA	15	0.1
(2,1870)	1:8:A:ILE:HG12	1:8:A:ILE:HA	17	0.1
(2,1860)	1:45:A:LYS:HB2	1:117:A:SER:HB2	19	0.1
(2,1787)	1:120:A:PHE:HE2	1:17:A:SER:HB3	16	0.1
(2,1731)	1:56:A:ILE:HG22	1:24:A:ILE:HA	3	0.1
(2,1654)	1:41:A:TYR:HB3	1:36:A:LEU:H	13	0.1
(2,1629)	1:77:A:GLY:HA2	1:105:A:ASN:HD21	6	0.1
(2,1523)	1:63:A:LEU:HG	1:62:A:SER:H	17	0.1
(2,1440)	1:20:A:GLU:HG2	1:35:A:ARG:HE	6	0.1
(2,1401)	1:106:A:VAL:HG11	1:105:A:ASN:HD22	9	0.1
(2,1324)	1:100:A:SER:HB3	1:101:A:ASN:HD22	9	0.1
(2,1229)	1:130:A:THR:HG21	1:130:A:THR:H	10	0.1
(2,1229)	1:130:A:THR:HG22	1:130:A:THR:H	10	0.1
(2,1229)	1:130:A:THR:HG23	1:130:A:THR:H	10	0.1
(2,1229)	1:130:A:THR:HG21	1:130:A:THR:H	15	0.1
(2,1229)	1:130:A:THR:HG22	1:130:A:THR:H	15	0.1
(2,1229)	1:130:A:THR:HG23	1:130:A:THR:H	15	0.1
(2,1222)	1:33:A:LYS:HD2	1:41:A:TYR:H	1	0.1
(2,1196)	1:45:A:LYS:HB2	1:47:A:ASP:H	14	0.1
(2,1188)	1:37:A:ASN:HB2	1:15:A:SER:H	17	0.1
(2,1030)	1:22:A:VAL:HB	1:29:A:ASP:H	9	0.1
(2,1030)	1:22:A:VAL:HB	1:29:A:ASP:H	11	0.1
(2,1019)	1:118:A:LEU:HB3	1:66:A:ILE:H	12	0.1
(2,1017)	1:45:A:LYS:HD2	1:117:A:SER:H	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1016)	1:45:A:LYS:HB3	1:117:A:SER:H	16	0.1
(2,980)	1:141:A:HIS:HB2	1:141:A:HIS:H	13	0.1
(2,980)	1:141:A:HIS:HB2	1:141:A:HIS:H	17	0.1
(2,886)	1:24:A:ILE:HG22	1:26:A:ASP:H	4	0.1
(2,886)	1:28:A:LEU:HD11	1:26:A:ASP:H	13	0.1
(2,871)	1:119:A:ILE:HD11	1:119:A:ILE:H	2	0.1
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	5	0.1
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	5	0.1
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	5	0.1
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	10	0.1
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	10	0.1
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	10	0.1
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	14	0.1
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	14	0.1
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	14	0.1
(2,847)	1:118:A:LEU:HD21	1:118:A:LEU:H	15	0.1
(2,847)	1:118:A:LEU:HD22	1:118:A:LEU:H	15	0.1
(2,847)	1:118:A:LEU:HD23	1:118:A:LEU:H	15	0.1
(2,844)	1:94:A:LEU:HD21	1:94:A:LEU:H	17	0.1
(2,808)	1:11:A:LYS:HD2	1:12:A:ASP:H	15	0.1
(2,808)	1:11:A:LYS:HD3	1:12:A:ASP:H	15	0.1
(2,803)	1:98:A:GLU:HG3	1:98:A:GLU:H	12	0.1
(2,799)	1:138:A:MET:HB2	1:139:A:LEU:H	1	0.1
(2,799)	1:138:A:MET:HB3	1:139:A:LEU:H	1	0.1
(2,771)	1:26:A:ASP:HB3	1:26:A:ASP:H	9	0.1
(2,700)	1:140:A:GLU:HA	1:140:A:GLU:H	1	0.1
(2,700)	1:140:A:GLU:HA	1:140:A:GLU:H	2	0.1
(2,700)	1:140:A:GLU:HA	1:140:A:GLU:H	11	0.1
(2,700)	1:140:A:GLU:HA	1:140:A:GLU:H	14	0.1
(2,700)	1:140:A:GLU:HA	1:140:A:GLU:H	15	0.1
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	14	0.1
(2,512)	1:107:A:ASP:HB3	1:107:A:ASP:H	16	0.1
(2,492)	1:70:A:PHE:HB3	1:79:A:TYR:H	15	0.1
(2,401)	1:70:A:PHE:HE1	1:69:A:ILE:H	16	0.1
(2,294)	1:127:A:ARG:HA	1:127:A:ARG:H	14	0.1
(2,293)	1:129:A:TYR:HA	1:129:A:TYR:H	20	0.1
(2,255)	1:93:A:ILE:HG12	1:93:A:ILE:H	10	0.1
(2,225)	1:98:A:GLU:HG2	1:99:A:ILE:H	1	0.1
(2,195)	1:92:A:SER:HA	1:99:A:ILE:H	8	0.1
(2,158)	1:123:A:LEU:HD23	1:123:A:LEU:H	2	0.1
(2,150)	1:22:A:VAL:HB	1:31:A:LYS:H	7	0.1
(2,130)	1:79:A:TYR:HB3	1:70:A:PHE:H	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,112)	1:31:A:LYS:HA	1:31:A:LYS:H	9	0.1
(2,95)	1:70:A:PHE:HD1	1:122:A:ILE:H	13	0.1
(2,34)	1:71:A:ILE:HG23	1:72:A:LYS:H	4	0.1
(2,29)	1:48:A:GLU:HG3	1:46:A:LYS:H	17	0.1
(2,5)	1:64:A:VAL:HA	1:86:A:TRP:HE1	2	0.1

10 Dihedral-angle violation analysis [i](#)

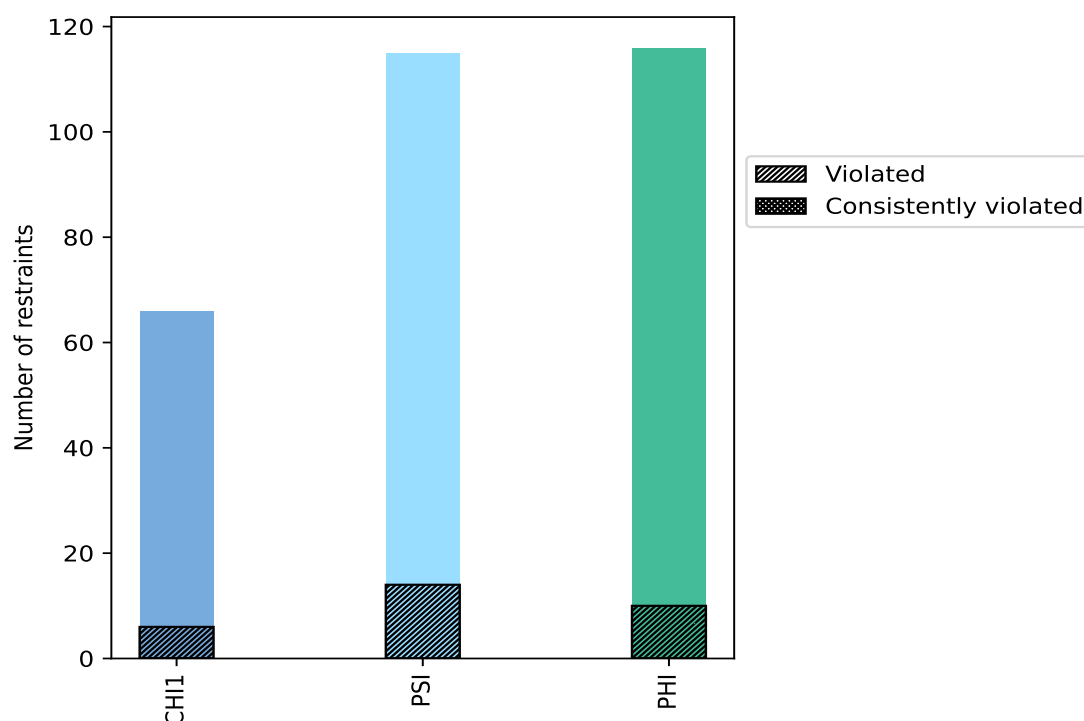
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
CHI1	66	22.2	6	9.1	2.0	0	0.0	0.0
PSI	115	38.7	14	12.2	4.7	0	0.0	0.0
PHI	116	39.1	10	8.6	3.4	0	0.0	0.0
Total	297	100.0	30	10.1	10.1	0	0.0	0.0

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



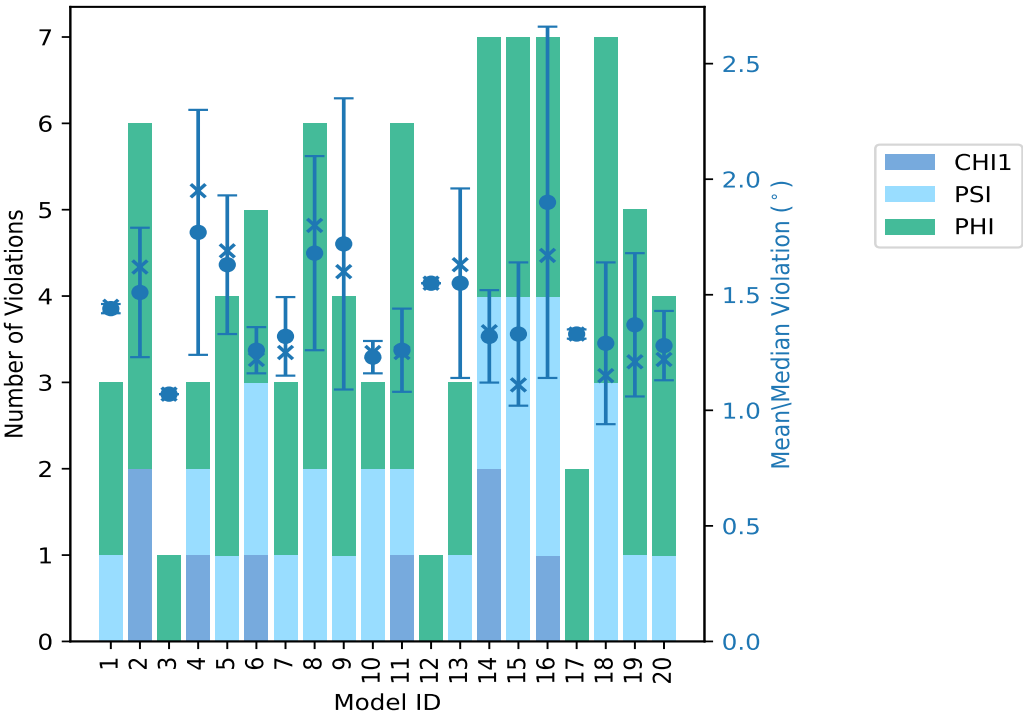
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations				Mean (°)	Max (°)	SD (°)	Median (°)
	CHI1	PSI	PHI	Total				
1	0	1	2	3	1.44	1.47	0.02	1.45
2	2	0	4	6	1.51	1.81	0.28	1.62
3	0	0	1	1	1.07	1.07	0.0	1.07
4	1	1	1	3	1.77	2.32	0.53	1.95
5	0	1	3	4	1.63	1.94	0.3	1.69
6	1	2	2	5	1.26	1.42	0.1	1.22
7	0	1	2	3	1.32	1.55	0.17	1.25
8	0	2	4	6	1.68	2.19	0.42	1.8
9	0	1	3	4	1.72	2.62	0.63	1.6
10	0	2	1	3	1.23	1.3	0.07	1.25
11	1	1	4	6	1.26	1.52	0.18	1.25
12	0	0	1	1	1.55	1.55	0.0	1.55
13	0	1	2	3	1.55	2.01	0.41	1.63
14	2	2	3	7	1.32	1.66	0.2	1.34
15	0	4	3	7	1.33	1.8	0.31	1.11
16	1	3	3	7	1.9	3.57	0.76	1.67
17	0	0	2	2	1.33	1.35	0.02	1.33
18	0	3	4	7	1.29	2.1	0.35	1.15
19	0	1	4	5	1.37	1.82	0.31	1.21
20	0	1	3	4	1.28	1.54	0.15	1.22

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints				Fraction of the ensemble	
CHI1	PSI	PHI	Total	Count ¹	%
4	6	4	14	1	5.0
2	4	1	7	2	10.0
0	3	1	4	3	15.0
0	1	0	1	4	20.0
0	0	1	1	5	25.0
0	0	1	1	6	30.0
0	0	0	0	7	35.0
0	0	0	0	8	40.0
0	0	0	0	9	45.0
0	0	0	0	10	50.0
0	0	0	0	11	55.0

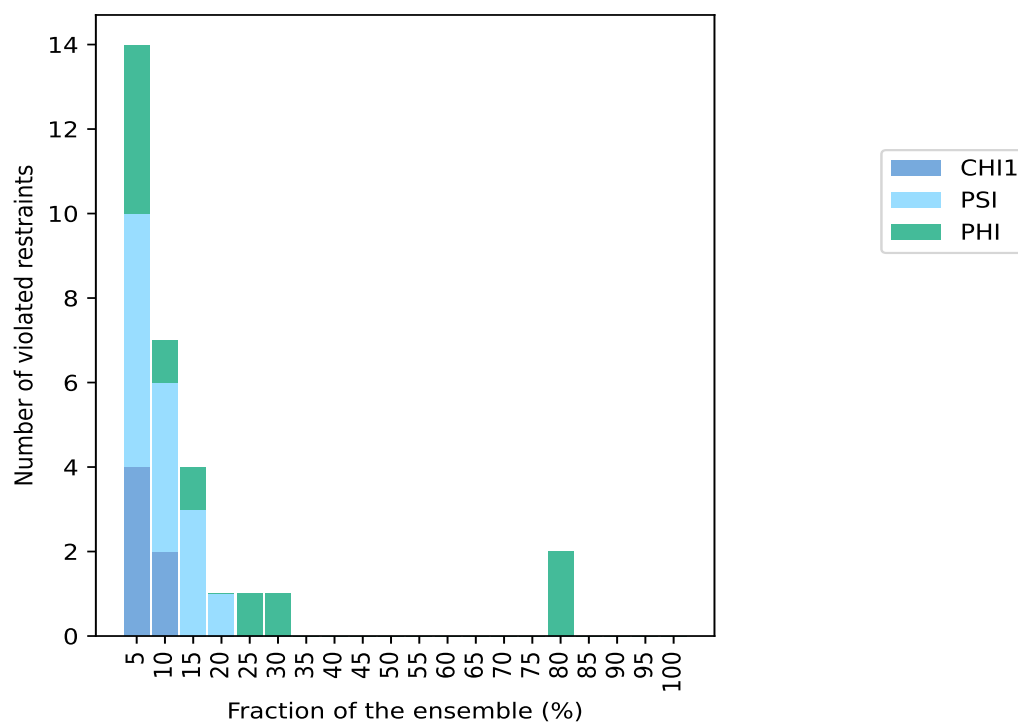
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Number of violated restraints				Fraction of the ensemble	
CHI1	PSI	PHI	Total	Count ¹	%
0	0	0	0	12	60.0
0	0	0	0	13	65.0
0	0	0	0	14	70.0
0	0	0	0	15	75.0
0	0	2	2	16	80.0
0	0	0	0	17	85.0
0	0	0	0	18	90.0
0	0	0	0	19	95.0
0	0	0	0	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)

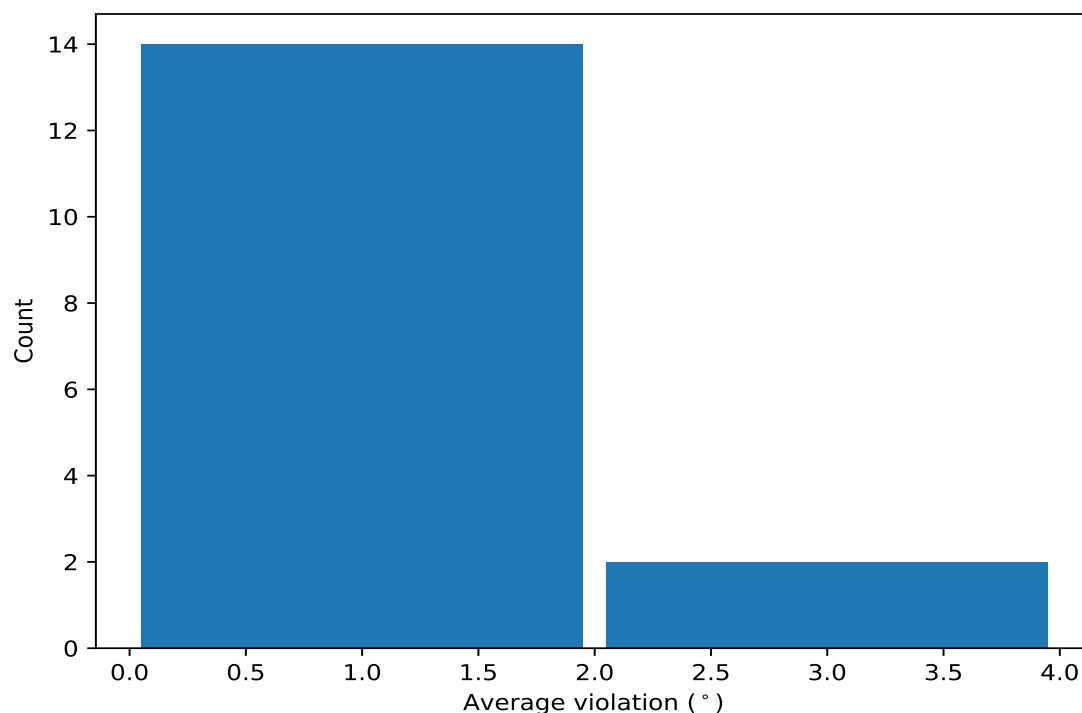


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle 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.

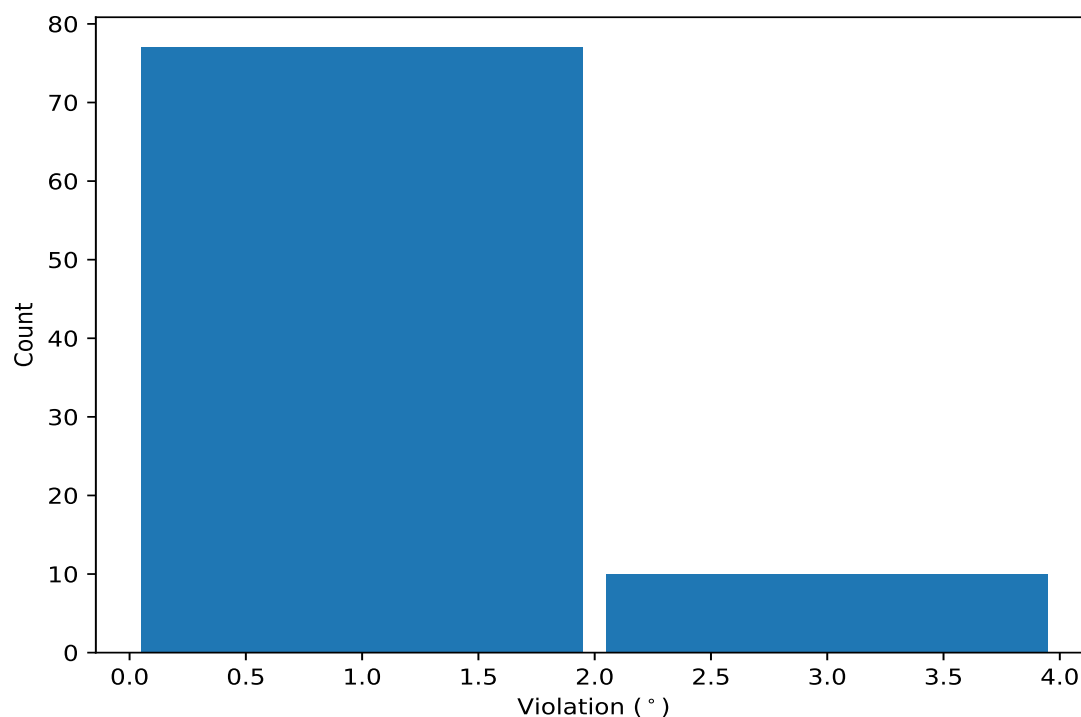
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	16	1.65	0.34	1.68
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	16	1.52	0.41	1.44
(1,164)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	6	1.36	0.35	1.22
(1,90)	1:55:A:ARG:C	1:56:A:ILE:N	1:56:A:ILE:CA	1:56:A:ILE:C	5	1.4	0.18	1.34
(1,165)	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	1:99:A:ILE:N	4	1.2	0.18	1.14
(1,45)	1:33:A:LYS:N	1:33:A:LYS:CA	1:33:A:LYS:C	1:34:A:ILE:N	3	1.4	0.19	1.32
(1,229)	1:139:A:LEU:N	1:139:A:LEU:CA	1:139:A:LEU:C	1:140:A:GLU:N	3	1.25	0.2	1.22
(1,231)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:HIS:N	3	1.17	0.12	1.15
(1,13)	1:16:A:SER:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	3	1.1	0.07	1.06
(1,226)	1:137:A:GLU:C	1:138:A:MET:N	1:138:A:MET:CA	1:138:A:MET:C	2	2.73	0.84	2.73
(1,277)	1:101:A:ASN:N	1:101:A:ASN:CA	1:101:A:ASN:CB	1:101:A:ASN:CG	2	2.16	0.16	2.16
(1,125)	1:74:A:SER:N	1:74:A:SER:CA	1:74:A:SER:C	1:75:A:GLU:N	2	1.62	0.48	1.62
(1,255)	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:CB	1:59:A:TYR:CG	2	1.26	0.08	1.26
(1,111)	1:67:A:PRO:N	1:67:A:PRO:CA	1:67:A:PRO:C	1:68:A:PHE:N	2	1.22	0.03	1.22
(1,191)	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	1:114:A:GLU:N	2	1.1	0.03	1.1
(1,137)	1:83:A:GLY:N	1:83:A:GLY:CA	1:83:A:GLY:C	1:84:A:GLU:N	2	1.06	0.02	1.06

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,226)	1:137:A:GLU:C	1:138:A:MET:N	1:138:A:MET:CA	1:138:A:MET:C	16	3.57
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	9	2.62
(1,277)	1:101:A:ASN:N	1:101:A:ASN:CA	1:101:A:ASN:CB	1:101:A:ASN:CG	4	2.32
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	16	2.21
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	8	2.19
(1,125)	1:74:A:SER:N	1:74:A:SER:CA	1:74:A:SER:C	1:75:A:GLU:N	18	2.1
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	8	2.04
(1,277)	1:101:A:ASN:N	1:101:A:ASN:CA	1:101:A:ASN:CB	1:101:A:ASN:CG	16	2.01
(1,164)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	13	2.01
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	9	2.0
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	4	1.95
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	5	1.94
(1,226)	1:137:A:GLU:C	1:138:A:MET:N	1:138:A:MET:CA	1:138:A:MET:C	8	1.89
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	5	1.87

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	19	1.82
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	2	1.81
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	15	1.8
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	15	1.75
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	2	1.73
(1,225)	1:137:A:GLU:N	1:137:A:GLU:CA	1:137:A:GLU:C	1:138:A:MET:N	8	1.72
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	16	1.67
(1,90)	1:55:A:ARG:C	1:56:A:ILE:N	1:56:A:ILE:CA	1:56:A:ILE:C	2	1.66
(1,45)	1:33:A:LYS:N	1:33:A:LYS:CA	1:33:A:LYS:C	1:34:A:ILE:N	14	1.66
(1,162)	1:96:A:GLY:C	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	19	1.65
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	13	1.63
(1,164)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	2	1.58
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	7	1.55
(1,90)	1:55:A:ARG:C	1:56:A:ILE:N	1:56:A:ILE:CA	1:56:A:ILE:C	12	1.55
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	20	1.54
(1,275)	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:CB	1:97:A:ARG:CG	11	1.52
(1,229)	1:139:A:LEU:N	1:139:A:LEU:CA	1:139:A:LEU:C	1:140:A:GLU:N	5	1.51
(1,250)	1:41:A:TYR:N	1:41:A:TYR:CA	1:41:A:TYR:CB	1:41:A:TYR:CG	14	1.5
(1,165)	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	1:99:A:ILE:N	15	1.48
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	1	1.47
(1,167)	1:99:A:ILE:N	1:99:A:ILE:CA	1:99:A:ILE:C	1:100:A:SER:N	1	1.45
(1,239)	1:21:A:TYR:N	1:21:A:TYR:CA	1:21:A:TYR:CB	1:21:A:TYR:CG	6	1.42
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	11	1.42
(1,130)	1:79:A:TYR:C	1:80:A:PHE:N	1:80:A:PHE:CA	1:80:A:PHE:C	1	1.41
(1,228)	1:138:A:MET:C	1:139:A:LEU:N	1:139:A:LEU:CA	1:139:A:LEU:C	18	1.38
(1,164)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	17	1.35
(1,255)	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:CB	1:59:A:TYR:CG	14	1.34
(1,90)	1:55:A:ARG:C	1:56:A:ILE:N	1:56:A:ILE:CA	1:56:A:ILE:C	14	1.34
(1,231)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:HIS:N	16	1.32
(1,45)	1:33:A:LYS:N	1:33:A:LYS:CA	1:33:A:LYS:C	1:34:A:ILE:N	16	1.32
(1,10)	1:15:A:SER:N	1:15:A:SER:CA	1:15:A:SER:C	1:16:A:SER:N	6	1.32
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	17	1.31
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	10	1.3
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	11	1.3
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	18	1.26
(1,111)	1:67:A:PRO:N	1:67:A:PRO:CA	1:67:A:PRO:C	1:68:A:PHE:N	10	1.25
(1,90)	1:55:A:ARG:C	1:56:A:ILE:N	1:56:A:ILE:CA	1:56:A:ILE:C	20	1.25
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	7	1.25
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	14	1.23
(1,229)	1:139:A:LEU:N	1:139:A:LEU:CA	1:139:A:LEU:C	1:140:A:GLU:N	16	1.22
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	6	1.22
(1,196)	1:115:A:TYR:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	6	1.21
(1,45)	1:33:A:LYS:N	1:33:A:LYS:CA	1:33:A:LYS:C	1:34:A:ILE:N	11	1.21
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	19	1.21
(1,165)	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	1:99:A:ILE:N	9	1.19
(1,111)	1:67:A:PRO:N	1:67:A:PRO:CA	1:67:A:PRO:C	1:68:A:PHE:N	20	1.19
(1,90)	1:55:A:ARG:C	1:56:A:ILE:N	1:56:A:ILE:CA	1:56:A:ILE:C	5	1.19
(1,13)	1:16:A:SER:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	8	1.19
(1,255)	1:59:A:TYR:N	1:59:A:TYR:CA	1:59:A:TYR:CB	1:59:A:TYR:CG	2	1.18
(1,231)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:HIS:N	7	1.15
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	18	1.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	20	1.15
(1,125)	1:74:A:SER:N	1:74:A:SER:CA	1:74:A:SER:C	1:75:A:GLU:N	10	1.14
(1,191)	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	1:114:A:GLU:N	6	1.13
(1,59)	1:40:A:PHE:N	1:40:A:PHE:CA	1:40:A:PHE:C	1:41:A:TYR:N	15	1.11
(1,165)	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	1:99:A:ILE:N	19	1.09
(1,164)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	9	1.09
(1,264)	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:CB	1:76:A:ILE:CG1	2	1.08
(1,137)	1:83:A:GLY:N	1:83:A:GLY:CA	1:83:A:GLY:C	1:84:A:GLU:N	14	1.08
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	14	1.08
(1,8)	1:14:A:PHE:N	1:14:A:PHE:CA	1:14:A:PHE:C	1:15:A:SER:N	15	1.08
(1,191)	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	1:114:A:GLU:N	8	1.07
(1,164)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	15	1.07
(1,39)	1:29:A:ASP:C	1:30:A:GLY:N	1:30:A:GLY:CA	1:30:A:GLY:C	3	1.07
(1,102)	1:61:A:TRP:C	1:62:A:SER:N	1:62:A:SER:CA	1:62:A:SER:C	11	1.06
(1,65)	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	1:44:A:ILE:N	18	1.06
(1,13)	1:16:A:SER:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	19	1.06
(1,137)	1:83:A:GLY:N	1:83:A:GLY:CA	1:83:A:GLY:C	1:84:A:GLU:N	4	1.05
(1,231)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:HIS:N	15	1.04
(1,13)	1:16:A:SER:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	18	1.04
(1,164)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	11	1.03
(1,229)	1:139:A:LEU:N	1:139:A:LEU:CA	1:139:A:LEU:C	1:140:A:GLU:N	18	1.02
(1,165)	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	1:99:A:ILE:N	13	1.02