



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 10:50 PM UTC

PDB ID : 8UOZ / pdb_00008uoz
BMRB ID : 31121
Title : EmrE structure in the TPP-bound state (WT/E14Q heterodimer)
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Deposited on : 2023-10-20

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

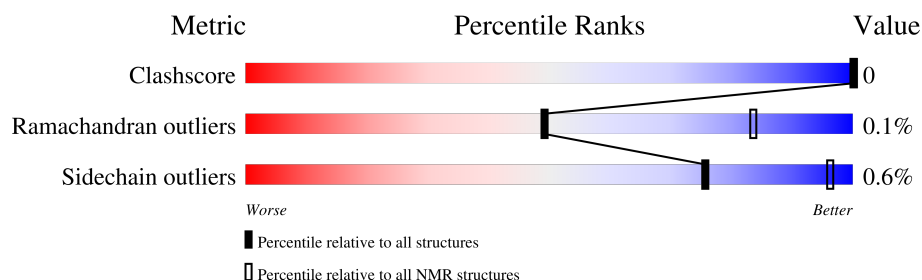
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 32%.

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	110	 95% 5%
2	B	110	 99% .

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:106, B:1-B:110 (215)	0.84	4

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3485 atoms, of which 1776 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SMR family multidrug efflux protein EmrE.

Mol	Chain	Residues	Atoms						Trace
1	A	110	Total	C	H	N	O	S	0
			1719	564	877	130	141	7	

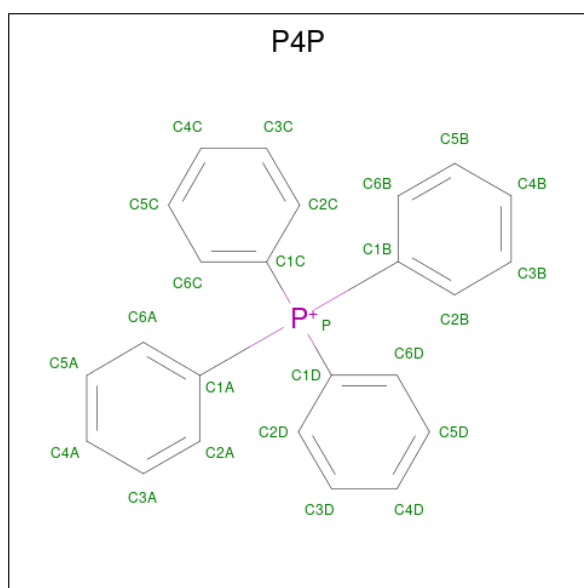
- Molecule 2 is a protein called SMR family multidrug efflux protein EmrE.

Mol	Chain	Residues	Atoms						Trace
2	B	110	Total	C	H	N	O	S	0
			1721	564	879	131	140	7	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLN	GLU	engineered mutation	UNP A0A2X7QID6

- Molecule 3 is TETRAPHENYLPHOSPHONIUM (CCD ID: P4P) (formula: $C_{24}H_{20}P$).



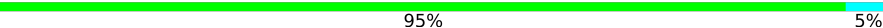
Mol	Chain	Residues	Atoms			
3	A	1	Total	C	H	P
			45	24	20	1

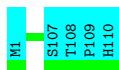
4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

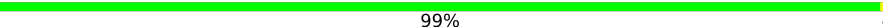
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for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

- Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:  95% 5%



- Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:  99%



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

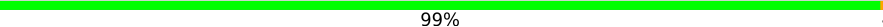
4.2.1 Score per residue for model 1

- Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:  95% 5%



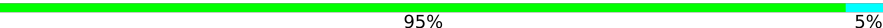
- Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:  99%



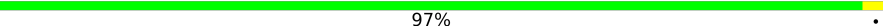
4.2.2 Score per residue for model 2

- Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:  95% 5%



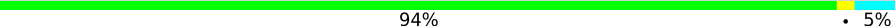
- Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:  97% .



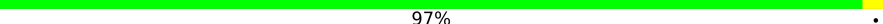
4.2.3 Score per residue for model 3

- Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:  94% . 5%



- Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:  97% .



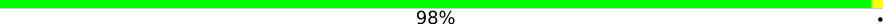
4.2.4 Score per residue for model 4 (medoid)

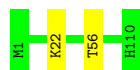
- Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:  94% . 5%



- Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:  98% .



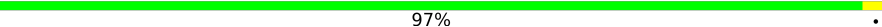
4.2.5 Score per residue for model 5

- Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:  95% 5%



- Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:  97% .



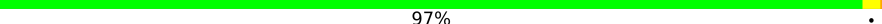
4.2.6 Score per residue for model 6

- Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:  95% 5%



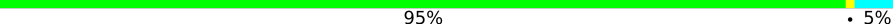
- Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:  97% ..



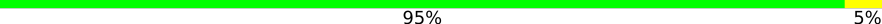
4.2.7 Score per residue for model 7

- Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:  95% 5%



- Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:  95% 5%



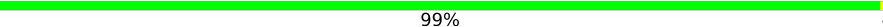
4.2.8 Score per residue for model 8

- Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:  93% 5%



- Molecule 2: SMR family multidrug efflux protein EmrE

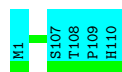
Chain B:  99%



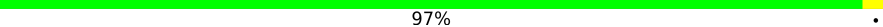
4.2.9 Score per residue for model 9

- Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:  95% 5%



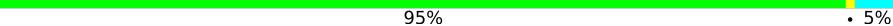
- Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:  97%



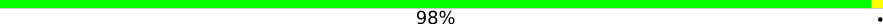
4.2.10 Score per residue for model 10

- Molecule 1: SMR family multidrug efflux protein EmrE

Chain A:  95% 5%



- Molecule 2: SMR family multidrug efflux protein EmrE

Chain B:  98%



5 Refinement protocol and experimental data overview

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

Of the 100000 calculated structures, 10 were deposited, based on the following criterion: *back calculated data agree with experimental NMR data*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
GROMACS	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	980
Number of shifts mapped to atoms	980
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	32%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P4P

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	0.88±0.01	0±0/825 (0.0± 0.0%)	1.54±0.02	1±1/1128 (0.1± 0.1%)
2	B	0.88±0.01	0±0/865 (0.0± 0.0%)	1.59±0.01	2±2/1180 (0.2± 0.2%)
All	All	0.88	0/16900 (0.0%)	1.56	31/23080 (0.1%)

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±0.5
2	B	0.0±0.0	0.2±0.4
All	All	0	5

There are no bond-length outliers.

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
2	B	2	ASN	CA-CB-CG	8.53	121.13	112.60	6	1
2	B	2	ASN	CB-CA-C	5.77	118.56	109.27	6	1
2	B	56	THR	N-CA-C	5.75	117.22	111.07	2	3
2	B	79	PHE	CA-CB-CG	-5.58	108.22	113.80	7	2
2	B	108	THR	CA-C-N	5.58	126.81	119.84	9	1
2	B	108	THR	C-N-CA	5.58	126.81	119.84	9	1
2	B	30	LEU	N-CA-C	5.52	116.97	111.07	2	1
2	B	22	LYS	N-CA-C	5.50	116.96	111.07	4	1
2	B	31	TRP	CA-C-N	5.40	124.85	119.24	9	1
2	B	31	TRP	C-N-CA	5.40	124.85	119.24	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	76	TRP	CA-C-N	5.36	125.89	119.94	8	1
1	A	76	TRP	C-N-CA	5.36	125.89	119.94	8	1
2	B	106	ARG	N-CA-C	5.35	117.11	111.28	3	1
2	B	84	ASP	CA-C-N	5.31	126.73	120.09	7	1
2	B	84	ASP	C-N-CA	5.31	126.73	120.09	7	1
2	B	2	ASN	CA-C-N	5.21	124.66	119.24	5	1
2	B	2	ASN	C-N-CA	5.21	124.66	119.24	5	1
2	B	16	ILE	CA-C-N	5.17	125.69	120.00	7	1
2	B	16	ILE	C-N-CA	5.17	125.69	120.00	7	1
1	A	31	TRP	CA-C-N	5.14	124.58	119.24	4	1
1	A	31	TRP	C-N-CA	5.14	124.58	119.24	4	1
2	B	51	LEU	N-CA-C	5.13	116.87	111.28	7	1
2	B	50	THR	CA-C-N	5.11	127.12	120.28	6	1
2	B	50	THR	C-N-CA	5.11	127.12	120.28	6	1
1	A	96	ALA	CA-C-N	5.08	125.58	119.94	3	1
1	A	96	ALA	C-N-CA	5.08	125.58	119.94	3	1
1	A	54	ILE	CA-C-N	5.05	125.04	119.89	8	1
1	A	54	ILE	C-N-CA	5.05	125.04	119.89	8	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)
2	B	60	TYR	Sidechain	1
2	B	29	ARG	Sidechain	1
1	A	4	TYR	Sidechain	1
1	A	106	ARG	Sidechain	1
1	A	29	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	803	840	840	0±0
2	B	842	879	879	0±0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	16700	17390	17390	-

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 -.

There are no clashes.

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	105/110 (95%)	102±1 (97±1%)	3±1 (3±1%)	0±0 (0±0%)	49 83
2	B	108/110 (98%)	105±1 (97±1%)	3±1 (3±1%)	0±0 (0±0%)	44 80
All	All	2130/2200 (97%)	2068 (97%)	59 (3%)	3 (0%)	49 83

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	25	GLU	2
1	A	27	PHE	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	84/89 (94%)	84±0 (100±1%)	0±0 (0±1%)	81 97
2	B	89/89 (100%)	88±1 (99±1%)	1±1 (1±1%)	70 95
All	All	1730/1780 (97%)	1720 (99%)	10 (1%)	76 96

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

Mol	Chain	Res	Type	Models (Total)
2	B	56	THR	3
2	B	81	GLN	3
1	A	56	THR	1
1	A	12	LEU	1
2	B	2	ASN	1
1	A	93	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	P4P	A	201	-	28,28,28	2.16±0.04	12±0 (42±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard

deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	P4P	A	201	-	38,38,38	1.52±0.07	6±1 (14±3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P4P	A	201	-	-	0±0,24,24,24	0±0,4,4,4

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
3	A	201	P4P	P-C1B	4.18	1.87	1.79	6	10
3	A	201	P4P	P-C1D	4.14	1.87	1.79	7	10
3	A	201	P4P	P-C1A	3.91	1.86	1.79	2	10
3	A	201	P4P	P-C1C	3.78	1.86	1.79	1	10
3	A	201	P4P	C6C-C1C	3.73	1.45	1.39	2	10
3	A	201	P4P	C2C-C1C	3.54	1.45	1.39	10	10
3	A	201	P4P	C6A-C1A	3.48	1.44	1.39	4	10
3	A	201	P4P	C6D-C1D	3.45	1.44	1.39	5	10
3	A	201	P4P	C2D-C1D	3.41	1.44	1.39	4	10
3	A	201	P4P	C6B-C1B	3.31	1.44	1.39	8	10
3	A	201	P4P	C2B-C1B	3.17	1.44	1.39	2	10
3	A	201	P4P	C2A-C1A	3.15	1.44	1.39	6	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	201	P4P	C2C-C1C-C6C	3.84	114.15	118.93	1	10
3	A	201	P4P	C2B-C1B-C6B	3.53	114.53	118.93	8	10
3	A	201	P4P	C2D-C1D-C6D	3.51	114.55	118.93	5	10
3	A	201	P4P	C6A-C1A-C2A	3.31	114.80	118.93	3	10
3	A	201	P4P	C1D-P-C1A	3.10	115.68	109.43	2	1
3	A	201	P4P	C1C-P-C1A	2.85	103.69	109.43	2	1

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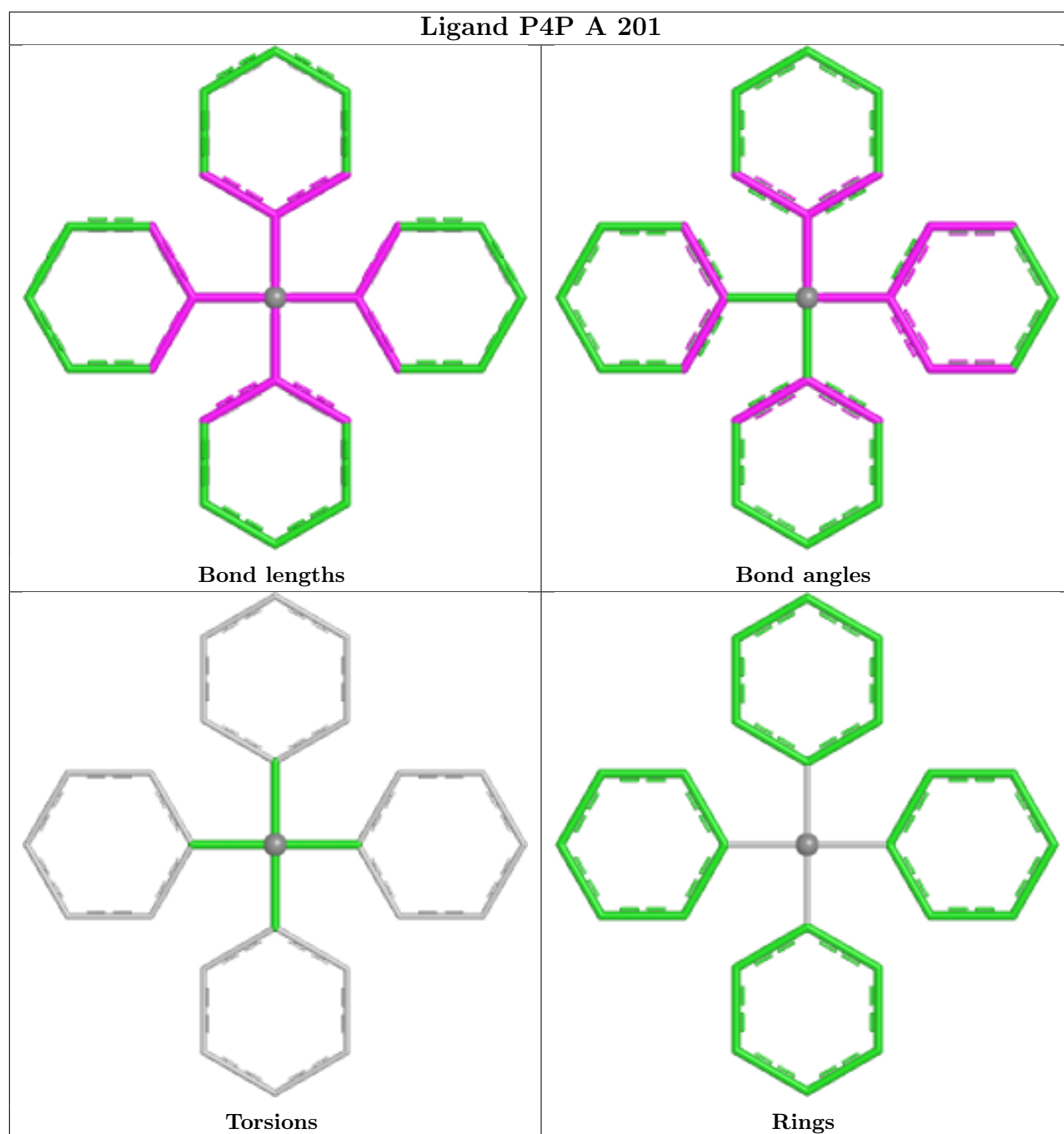
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	201	P4P	P-C1C-C2C	2.40	124.28	120.05	1	2
3	A	201	P4P	C3C-C2C-C1C	2.31	122.93	120.29	1	1
3	A	201	P4P	C1D-P-C1C	2.28	104.83	109.43	1	1
3	A	201	P4P	C5D-C6D-C1D	2.18	122.79	120.29	9	1
3	A	201	P4P	C5C-C6C-C1C	2.16	122.76	120.29	1	4
3	A	201	P4P	C1B-P-C1D	2.15	113.76	109.43	2	1
3	A	201	P4P	P-C1C-C6C	2.13	123.81	120.05	5	1
3	A	201	P4P	C3B-C2B-C1B	2.02	122.60	120.29	9	1
3	A	201	P4P	C3A-C2A-C1A	2.01	122.59	120.29	3	1
3	A	201	P4P	P-C1A-C6A	2.00	123.59	120.05	6	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 32% for the well-defined parts and 32% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	980
Number of shifts mapped to atoms	980
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	219	-0.83 ± 0.15	Should be checked
$^{13}\text{C}_\beta$	158	0.55 ± 0.08	Should be checked
$^{13}\text{C}'$	196	-0.47 ± 0.07	None needed (< 0.5 ppm)
^{15}N	206	0.63 ± 0.13	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 32%, i.e. 954 atoms were assigned a chemical shift out of a possible 2972. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	786/1081 (73%)	181/445 (41%)	407/430 (95%)	198/206 (96%)
Sidechain	153/1598 (10%)	0/1081 (0%)	153/488 (31%)	0/29 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	15/293 (5%)	10/142 (7%)	0/142 (0%)	5/9 (56%)
Overall	954/2972 (32%)	191/1668 (11%)	560/1060 (53%)	203/244 (83%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 32%, i.e. 974 atoms were assigned a chemical shift out of a possible 3033. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	801/1104 (73%)	184/454 (41%)	415/440 (94%)	202/210 (96%)
Sidechain	158/1629 (10%)	0/1102 (0%)	158/498 (32%)	0/29 (0%)
Aromatic	15/300 (5%)	10/146 (7%)	0/144 (0%)	5/10 (50%)
Overall	974/3033 (32%)	194/1702 (11%)	573/1082 (53%)	207/249 (83%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts ⓘ

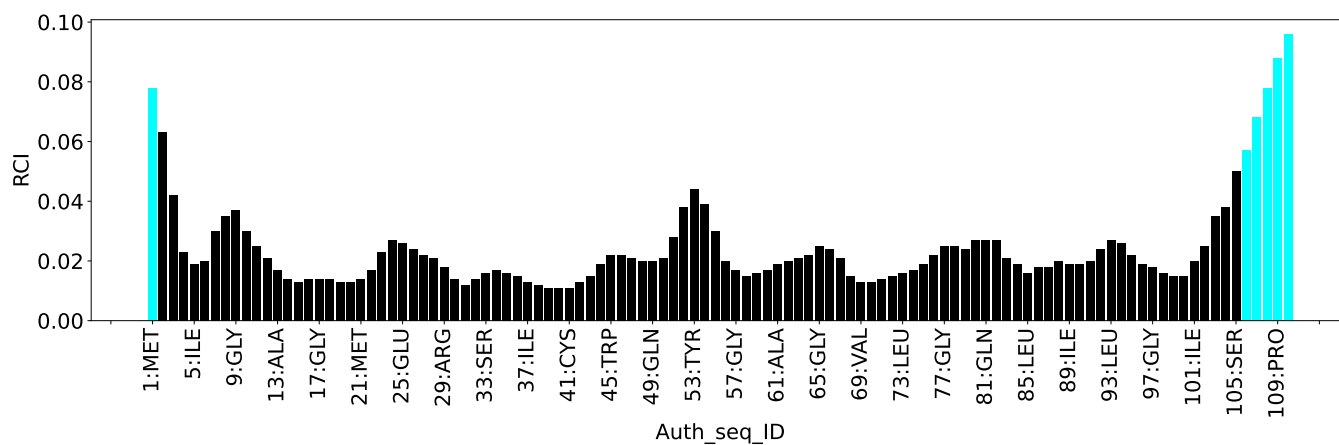
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	63	TRP	HE3	11.48	5.27 – 9.37	10.1
1	A	45	TRP	HE3	10.49	5.27 – 9.37	7.7
1	A	31	TRP	HE3	10.43	5.27 – 9.37	7.6
1	A	76	TRP	HE3	10.37	5.27 – 9.37	7.4

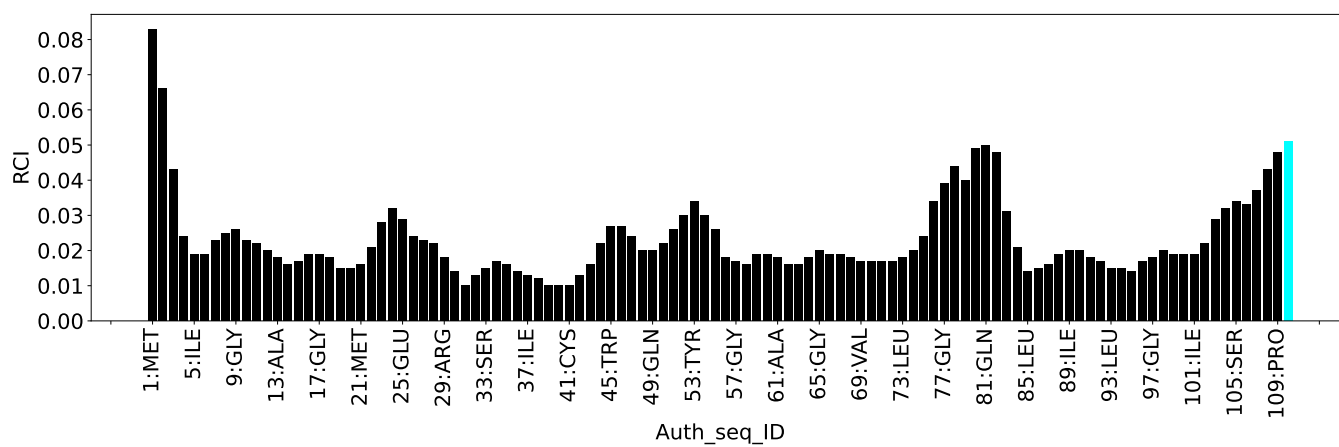
7.1.5 Random Coil Index (RCI) plots ⓘ

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:



Random coil index (RCI) for chain B:



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	1452
Intra-residue ($ i-j =0$)	1
Sequential ($ i-j =1$)	40
Medium range ($ i-j >1$ and $ i-j <5$)	131
Long range ($ i-j \geq 5$)	576
Inter-chain	488
Hydrogen bond restraints	216
Disulfide bond restraints	0
Total dihedral-angle restraints	390
Number of unmapped restraints	0
Number of restraints per residue	8.3
Number of long range restraints per residue ¹	2.6

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)	7.4	0.2
0.2-0.5 (Medium)	26.3	0.5
>0.5 (Large)	100.3	6.85

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)	11.5	9.64
10.0-20.0 (Medium)	5.6	19.87
>20.0 (Large)	7.1	158.86

9 Distance violation analysis ⓘ

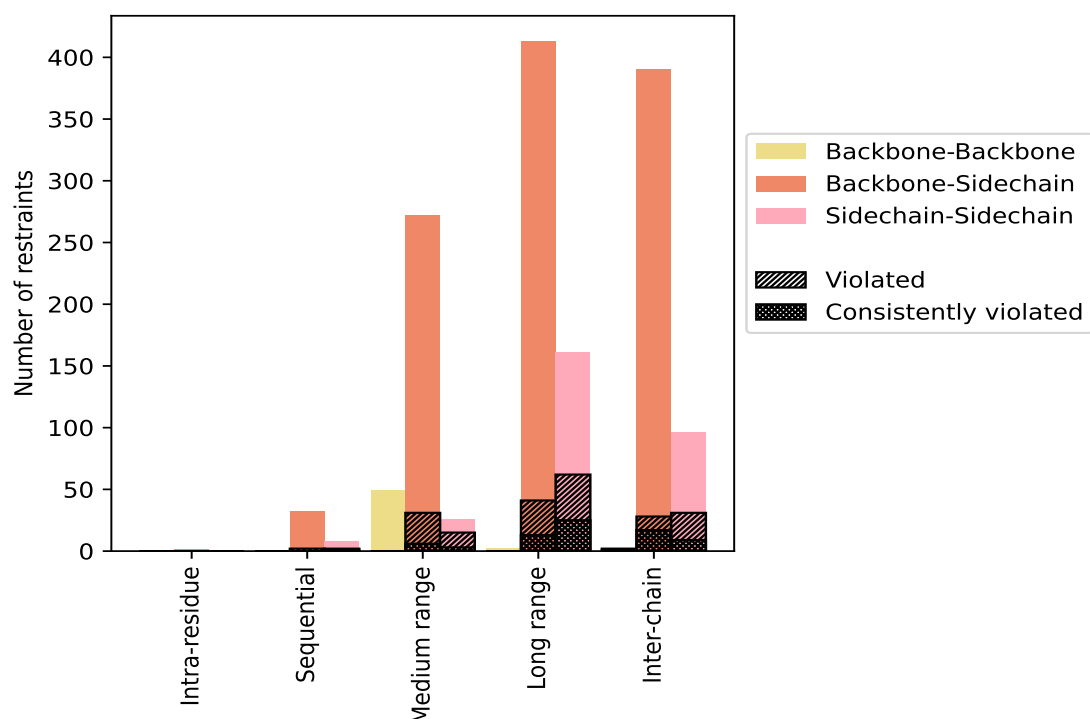
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	1	0.1	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	1	0.1	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
Sequential ($i-j =1$)	40	2.8	4	10.0	0.3	1	2.5	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	32	2.2	2	6.2	0.1	0	0.0	0.0
Sidechain-Sidechain	8	0.6	2	25.0	0.1	1	12.5	0.1
Medium range ($i-j >1$ & $i-j <5$)	131	9.0	22	16.8	1.5	5	3.8	0.3
Backbone-Backbone	49	3.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	56	3.9	7	12.5	0.5	2	3.6	0.1
Sidechain-Sidechain	26	1.8	15	57.7	1.0	3	11.5	0.2
Long range ($i-j \geq 5$)	576	39.7	103	17.9	7.1	38	6.6	2.6
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	413	28.4	41	9.9	2.8	13	3.1	0.9
Sidechain-Sidechain	161	11.1	62	38.5	4.3	25	15.5	1.7
Inter-chain	488	33.6	61	12.5	4.2	27	5.5	1.9
Backbone-Backbone	2	0.1	2	100.0	0.1	1	50.0	0.1
Backbone-Sidechain	390	26.9	28	7.2	1.9	17	4.4	1.2
Sidechain-Sidechain	96	6.6	31	32.3	2.1	9	9.4	0.6
Hydrogen bond	216	14.9	24	11.1	1.7	4	1.9	0.3
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1452	100.0	214	14.7	14.7	75	5.2	5.2
Backbone-Backbone	53	3.7	2	3.8	0.1	1	1.9	0.1
Backbone-Sidechain	1108	76.3	102	9.2	7.0	36	3.2	2.5
Sidechain-Sidechain	291	20.0	110	37.8	7.6	38	13.1	2.6

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

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



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

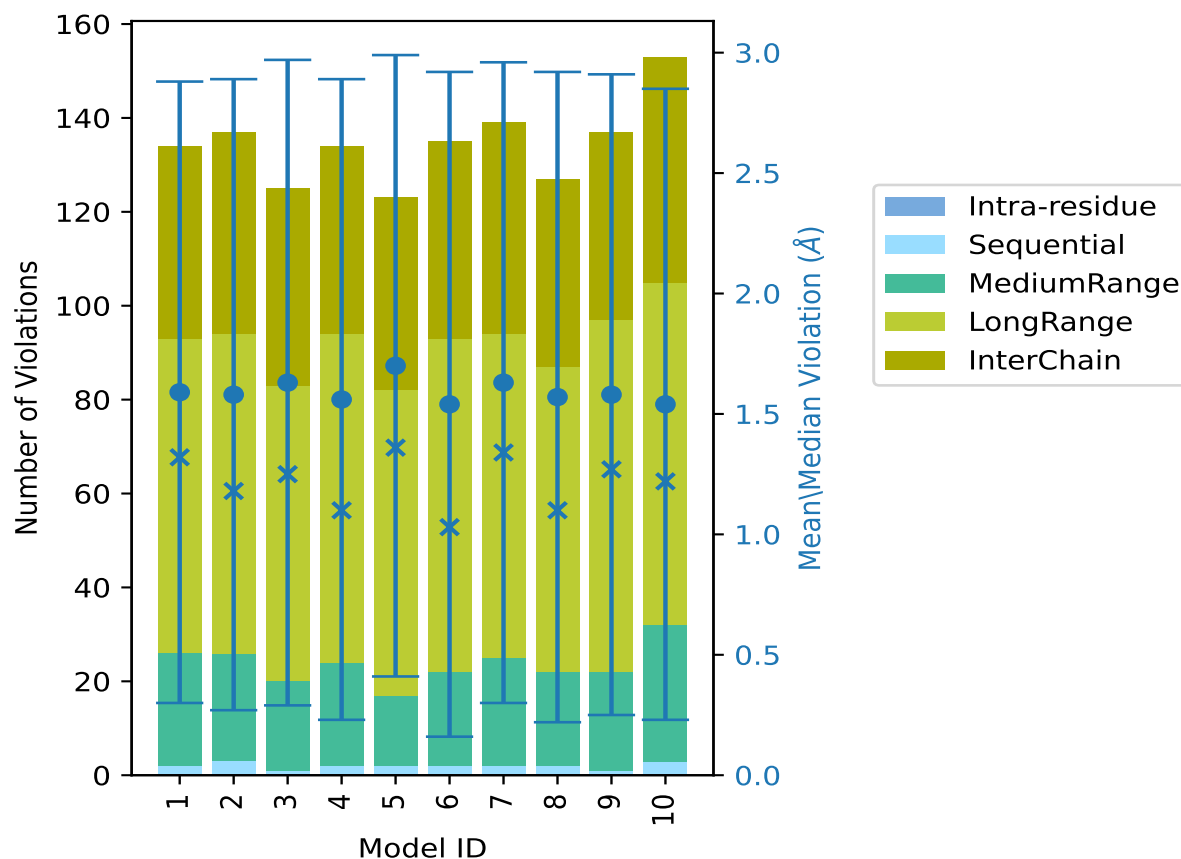
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	2	24	67	41	134	1.59	5.9	1.29	1.32
2	0	3	23	68	43	137	1.58	6.13	1.31	1.18
3	0	1	19	63	42	125	1.63	6.39	1.34	1.25
4	0	2	22	70	40	134	1.56	5.75	1.33	1.1
5	0	2	15	65	41	123	1.7	5.59	1.29	1.36
6	0	2	20	71	42	135	1.54	5.45	1.38	1.03
7	0	2	23	69	45	139	1.63	5.74	1.33	1.34
8	0	2	20	65	40	127	1.57	6.0	1.35	1.1
9	0	1	21	75	40	137	1.58	6.81	1.33	1.27
10	0	3	29	73	48	153	1.54	6.85	1.31	1.22

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1046(IR:1, SQ:36, MR:109, LR:473, IC:427) 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	%
0	2	5	9	3	19	1	10.0
0	0	1	10	4	15	2	20.0
0	0	3	11	9	23	3	30.0

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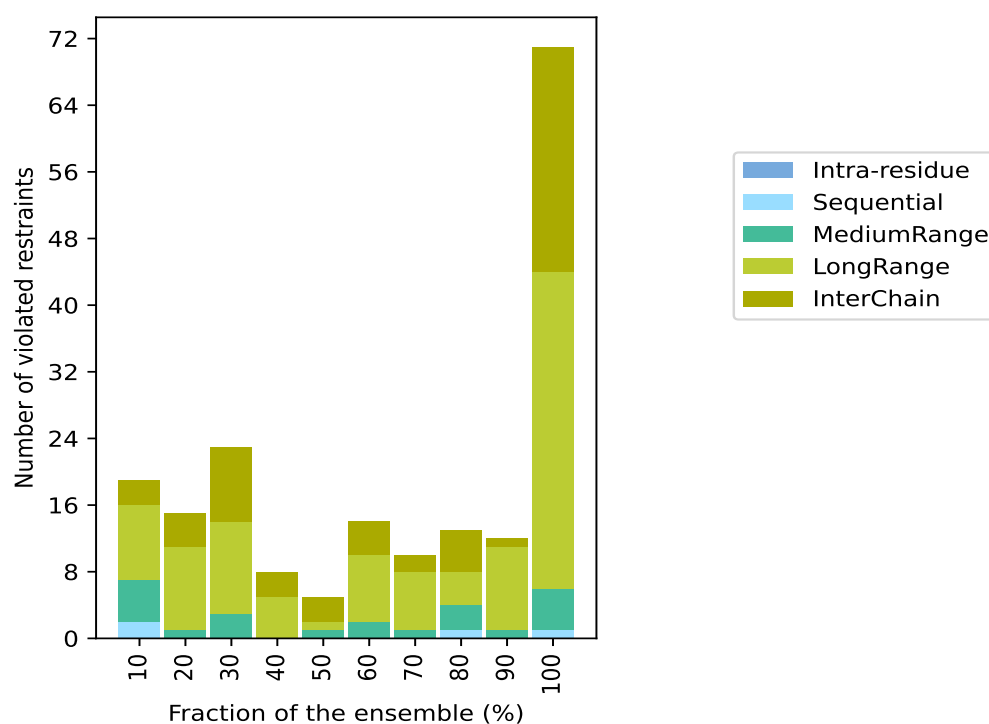
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	5	3	8	4	40.0
0	0	1	1	3	5	5	50.0
0	0	2	8	4	14	6	60.0
0	0	1	7	2	10	7	70.0
0	1	3	4	5	13	8	80.0
0	0	1	10	1	12	9	90.0
0	1	5	38	27	71	10	100.0

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

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

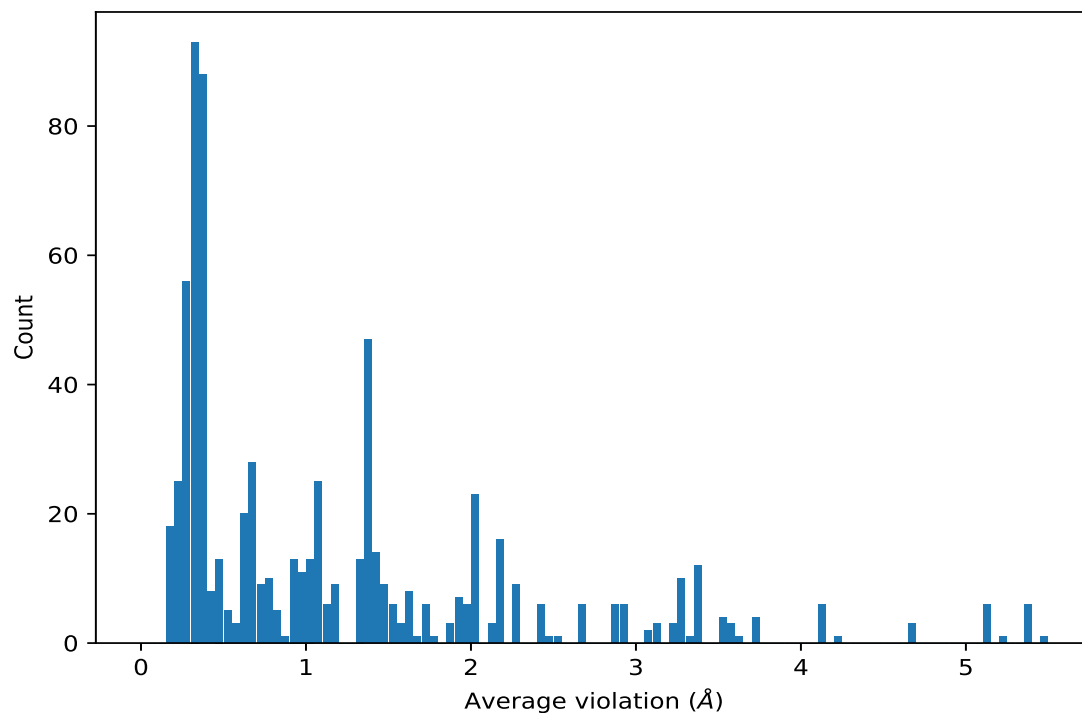


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	10	5.45	0.34	5.48
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	10	5.37	0.82	5.2
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	10	5.37	0.82	5.2
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	10	5.37	0.82	5.2
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	10	5.37	0.82	5.2
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	10	5.37	0.82	5.2
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	10	5.37	0.82	5.2
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	10	5.22	0.54	5.17
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	10	5.14	0.77	5.22
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	10	5.14	0.77	5.22
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	10	5.14	0.77	5.22
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	10	5.14	0.77	5.22
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	10	5.14	0.77	5.22
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	10	5.14	0.77	5.22
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	10	4.66	0.83	4.93

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	10	4.66	0.83	4.93
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	10	4.66	0.83	4.93
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	10	4.2	0.3	4.29
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	10	4.14	0.1	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	10	4.14	0.1	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	10	4.14	0.1	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	10	4.14	0.1	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	10	4.14	0.1	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	10	4.14	0.1	4.1
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	10	3.74	0.62	3.51
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	10	3.74	0.62	3.51
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	10	3.74	0.62	3.51
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	10	3.72	0.55	3.68
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	10	3.62	1.01	3.77
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD11	10	3.57	0.31	3.6
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD12	10	3.57	0.31	3.6
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD13	10	3.57	0.31	3.6
(2,72)	1:41:A:CYS:SG	2:4:B:TYR:H	10	3.55	0.38	3.5
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD11	10	3.54	0.45	3.55
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD12	10	3.54	0.45	3.55
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD13	10	3.54	0.45	3.55
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD11	10	3.37	0.47	3.54
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD12	10	3.37	0.47	3.54
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD13	10	3.37	0.47	3.54
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD21	10	3.37	0.47	3.54
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD22	10	3.37	0.47	3.54
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD23	10	3.37	0.47	3.54
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD11	10	3.36	0.38	3.51
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD12	10	3.36	0.38	3.51
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD13	10	3.36	0.38	3.51
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD21	10	3.36	0.38	3.51
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD22	10	3.36	0.38	3.51
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD23	10	3.36	0.38	3.51
(5,8)	2:94:B:ILE:CB	1:97:A:GLY:CA	10	3.32	0.31	3.34
(5,128)	1:80:A:GLY:CA	1:83:A:LEU:CG	10	3.3	0.29	3.29
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD11	10	3.28	0.45	3.27
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD12	10	3.28	0.45	3.27
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD13	10	3.28	0.45	3.27
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD11	10	3.26	0.28	3.22
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD12	10	3.26	0.28	3.22
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD13	10	3.26	0.28	3.22
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD21	10	3.26	0.28	3.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD22	10	3.26	0.28	3.22
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD23	10	3.26	0.28	3.22
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD11	10	3.22	0.51	3.18
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD12	10	3.22	0.51	3.18
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD13	10	3.22	0.51	3.18
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD11	10	3.15	0.42	3.28
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD12	10	3.15	0.42	3.28
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD13	10	3.15	0.42	3.28
(1,291)	2:39:B:CYS:SG	2:10:B:ALA:H	10	3.09	0.33	3.13
(2,34)	1:39:A:CYS:SG	2:56:B:THR:H	10	3.06	0.43	3.0
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD11	10	2.92	0.59	2.96
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD12	10	2.92	0.59	2.96
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD13	10	2.92	0.59	2.96
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD21	10	2.92	0.59	2.96
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD22	10	2.92	0.59	2.96
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD23	10	2.92	0.59	2.96
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD11	10	2.86	0.18	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD12	10	2.86	0.18	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD13	10	2.86	0.18	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD21	10	2.86	0.18	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD22	10	2.86	0.18	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD23	10	2.86	0.18	2.89
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD11	10	2.68	0.17	2.72
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD12	10	2.68	0.17	2.72
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD13	10	2.68	0.17	2.72
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD21	10	2.68	0.17	2.72
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD22	10	2.68	0.17	2.72
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD23	10	2.68	0.17	2.72
(5,63)	1:25:A:GLU:CD	1:22:A:LYS:CE	10	2.52	0.43	2.66
(2,38)	1:39:A:CYS:SG	2:60:B:TYR:H	10	2.46	0.44	2.4
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD11	10	2.41	0.76	2.45
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD12	10	2.41	0.76	2.45
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD13	10	2.41	0.76	2.45
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD21	10	2.41	0.76	2.45
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD22	10	2.41	0.76	2.45
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD23	10	2.41	0.76	2.45
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD11	10	2.28	0.34	2.32
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD12	10	2.28	0.34	2.32
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD13	10	2.28	0.34	2.32
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD21	10	2.28	0.34	2.32
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD22	10	2.28	0.34	2.32
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD23	10	2.28	0.34	2.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD11	10	2.18	0.96	2.1
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD12	10	2.18	0.96	2.1
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD13	10	2.18	0.96	2.1
(2,35)	1:39:A:CYS:SG	2:57:B:GLY:H	10	2.15	0.45	2.04
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD11	10	2.15	0.86	2.17
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD12	10	2.15	0.86	2.17
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD13	10	2.15	0.86	2.17
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD11	10	2.15	0.86	2.17
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD12	10	2.15	0.86	2.17
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD13	10	2.15	0.86	2.17
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD11	10	2.15	0.86	2.17
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD12	10	2.15	0.86	2.17
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD13	10	2.15	0.86	2.17
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD11	10	2.11	0.51	1.99
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD12	10	2.11	0.51	1.99
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD13	10	2.11	0.51	1.99
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD11	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD12	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD13	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD11	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD12	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD13	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD11	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD12	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD13	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD11	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD12	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD13	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD11	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD12	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD13	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD11	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD12	10	2.02	0.62	1.87
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD13	10	2.02	0.62	1.87
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD1	10	2.01	0.23	2.04
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD2	10	2.01	0.23	2.04
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD11	10	1.97	0.63	1.83
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD12	10	1.97	0.63	1.83
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD13	10	1.97	0.63	1.83
(1,304)	2:39:B:CYS:SG	2:33:B:SER:H	10	1.94	0.15	1.91
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD11	10	1.93	0.57	1.68
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD12	10	1.93	0.57	1.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD13	10	1.93	0.57	1.68
(1,97)	1:39:A:CYS:SG	1:75:A:SER:H	10	1.87	0.39	1.88
(1,300)	2:39:B:CYS:SG	2:28:B:THR:H	10	1.86	0.46	1.88
(2,36)	1:39:A:CYS:SG	2:58:B:ILE:H	10	1.79	0.4	1.65
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD11	10	1.74	0.59	1.59
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD12	10	1.74	0.59	1.59
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD13	10	1.74	0.59	1.59
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD21	10	1.74	0.59	1.59
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD22	10	1.74	0.59	1.59
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD23	10	1.74	0.59	1.59
(5,40)	2:63:B:TRP:CE2	2:62:B:ILE:CG2	10	1.68	0.11	1.64
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD11	10	1.64	0.86	1.5
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD12	10	1.64	0.86	1.5
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD13	10	1.64	0.86	1.5
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD21	10	1.64	0.86	1.5
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD22	10	1.64	0.86	1.5
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD23	10	1.64	0.86	1.5
(2,29)	1:39:A:CYS:SG	2:49:B:GLN:H	10	1.61	0.58	1.31
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD11	10	1.52	0.12	1.5
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD12	10	1.52	0.12	1.5
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD13	10	1.52	0.12	1.5
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD21	10	1.52	0.12	1.5
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD22	10	1.52	0.12	1.5
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD23	10	1.52	0.12	1.5
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD11	10	1.47	0.14	1.45
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD12	10	1.47	0.14	1.45
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD13	10	1.47	0.14	1.45
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD21	10	1.47	0.14	1.45
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD22	10	1.47	0.14	1.45
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD23	10	1.47	0.14	1.45
(2,75)	1:41:A:CYS:SG	2:8:B:GLY:H	10	1.44	0.21	1.53
(1,25)	1:5:A:ILE:CG1	1:54:A:ILE:H	10	1.42	0.38	1.41
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD11	10	1.39	0.52	1.57
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD12	10	1.39	0.52	1.57
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD13	10	1.39	0.52	1.57
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD21	10	1.39	0.52	1.57
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD22	10	1.39	0.52	1.57
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD23	10	1.39	0.52	1.57
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD11	10	1.33	0.34	1.27
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD12	10	1.33	0.34	1.27
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD13	10	1.33	0.34	1.27
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD11	10	1.33	0.34	1.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD12	10	1.33	0.34	1.27
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD13	10	1.33	0.34	1.27
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD11	10	1.33	0.34	1.27
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD12	10	1.33	0.34	1.27
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD13	10	1.33	0.34	1.27
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD11	10	1.3	0.54	1.42
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD12	10	1.3	0.54	1.42
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD13	10	1.3	0.54	1.42
(1,296)	2:39:B:CYS:SG	2:24:B:SER:H	10	1.18	0.4	1.11
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD11	10	1.09	0.71	0.82
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD12	10	1.09	0.71	0.82
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD13	10	1.09	0.71	0.82
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD11	10	1.07	0.25	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD12	10	1.07	0.25	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD13	10	1.07	0.25	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD21	10	1.07	0.25	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD22	10	1.07	0.25	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD23	10	1.07	0.25	1.08
(1,220)	1:95:A:CYS:SG	1:90:A:GLY:H	10	1.06	0.92	0.6
(2,30)	1:39:A:CYS:SG	2:51:B:LEU:H	10	1.06	0.44	1.01
(2,41)	1:39:A:CYS:SG	2:64:B:SER:H	10	0.99	0.43	0.99
(2,37)	1:39:A:CYS:SG	2:59:B:ALA:H	10	0.98	0.43	0.92
(2,205)	2:39:B:CYS:SG	1:37:A:ILE:H	10	0.96	0.3	0.9
(1,283)	2:5:B:ILE:CG1	2:105:B:SER:H	10	0.94	0.44	0.96
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD11	10	0.91	0.38	0.86
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD12	10	0.91	0.38	0.86
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD13	10	0.91	0.38	0.86
(6,67)	1:65:A:GLY:O	1:69:A:VAL:H	10	0.86	0.37	0.77
(5,134)	1:90:A:GLY:CA	1:86:A:PRO:CD	10	0.85	0.12	0.84
(2,28)	1:39:A:CYS:SG	2:43:B:SER:H	10	0.85	0.37	0.75
(2,209)	2:39:B:CYS:SG	1:44:A:PHE:H	10	0.83	0.34	0.84
(6,68)	1:69:A:VAL:N	1:65:A:GLY:O	10	0.8	0.35	0.72
(1,301)	2:39:B:CYS:SG	2:29:B:ARG:H	10	0.8	0.33	0.75
(2,27)	1:39:A:CYS:SG	2:40:B:TYR:H	10	0.72	0.27	0.7
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD11	10	0.71	0.33	0.77
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD12	10	0.71	0.33	0.77
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD13	10	0.71	0.33	0.77
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD21	10	0.71	0.33	0.77
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD22	10	0.71	0.33	0.77
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD23	10	0.71	0.33	0.77
(6,65)	1:64:A:SER:O	1:68:A:ILE:H	10	0.7	0.2	0.72
(5,5)	2:90:B:GLY:CA	1:97:A:GLY:CA	10	0.68	0.26	0.71

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(6,66)	1:68:A:ILE:N	1:64:A:SER:O	10	0.66	0.2	0.68
(1,303)	2:39:B:CYS:SG	2:31:B:TRP:H	10	0.51	0.27	0.46
(5,11)	2:25:B:GLU:CD	2:22:B:LYS:CE	9	1.86	1.09	1.76
(1,180)	1:95:A:CYS:SG	1:10:A:ALA:H	9	1.63	0.85	1.5
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD11	9	1.57	0.75	1.36
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD12	9	1.57	0.75	1.36
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD13	9	1.57	0.75	1.36
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD11	9	1.38	0.48	1.4
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD12	9	1.38	0.48	1.4
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD13	9	1.38	0.48	1.4
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD11	9	1.37	0.46	1.36
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD12	9	1.37	0.46	1.36
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD13	9	1.37	0.46	1.36
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD21	9	1.37	0.46	1.36
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD22	9	1.37	0.46	1.36
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD23	9	1.37	0.46	1.36
(1,179)	1:95:A:CYS:SG	1:9:A:GLY:H	9	1.36	0.84	0.94
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD11	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD12	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD13	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD21	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD22	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD23	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD11	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD12	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD13	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD21	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD22	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD23	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD11	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD12	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD13	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD21	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD22	9	1.35	0.79	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD23	9	1.35	0.79	1.03
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD11	9	1.06	0.37	1.19
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD12	9	1.06	0.37	1.19
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD13	9	1.06	0.37	1.19
(1,166)	1:41:A:CYS:SG	1:91:A:MET:H	9	0.79	0.37	0.8
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD11	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD12	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD13	9	0.62	0.4	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD11	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD12	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD13	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD11	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD12	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD13	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD11	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD12	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD13	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD11	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD12	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD13	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD11	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD12	9	0.62	0.4	0.41
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD13	9	0.62	0.4	0.41
(1,348)	2:95:B:CYS:SG	2:2:B:ASN:H	9	0.61	0.32	0.46
(5,95)	1:63:A:TRP:CA	1:14:A:GLU:CD	9	0.36	0.11	0.34
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD11	8	2.17	0.97	2.46
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD12	8	2.17	0.97	2.46
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD13	8	2.17	0.97	2.46
(3,33)	1:47:A:LEU:HD11	3:201:A:P4P:H2B	8	1.02	0.76	0.78
(3,33)	1:47:A:LEU:HD11	3:201:A:P4P:H2A	8	1.02	0.76	0.78
(3,33)	1:47:A:LEU:HD11	3:201:A:P4P:H2C	8	1.02	0.76	0.78
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD11	8	0.91	0.61	0.79
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD12	8	0.91	0.61	0.79
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD13	8	0.91	0.61	0.79
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD21	8	0.91	0.61	0.79
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD22	8	0.91	0.61	0.79
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD23	8	0.91	0.61	0.79
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD11	8	0.77	0.42	0.7
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD12	8	0.77	0.42	0.7
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD13	8	0.77	0.42	0.7
(1,369)	2:95:B:CYS:SG	2:40:B:TYR:H	8	0.72	0.4	0.56
(5,9)	2:10:B:ALA:CA	2:11:B:ILE:CD1	8	0.72	0.29	0.72
(1,298)	2:39:B:CYS:SG	2:26:B:GLY:H	8	0.7	0.5	0.56
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD11	8	0.65	0.42	0.56
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD12	8	0.65	0.42	0.56
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD13	8	0.65	0.42	0.56
(5,35)	2:28:B:THR:CB	2:30:B:LEU:CA	8	0.45	0.11	0.44
(5,81)	1:43:A:SER:CA	1:45:A:TRP:CD2	8	0.41	0.12	0.44
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD11	8	0.39	0.26	0.26
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD12	8	0.39	0.26	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD13	8	0.39	0.26	0.26
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD21	8	0.39	0.26	0.26
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD22	8	0.39	0.26	0.26
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD23	8	0.39	0.26	0.26
(1,284)	2:5:B:ILE:CG1	2:106:B:ARG:H	8	0.37	0.18	0.4
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD11	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD12	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD13	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD11	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD12	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD13	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD11	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD12	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD13	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD11	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD12	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD13	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD11	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD12	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD13	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD11	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD12	8	0.36	0.06	0.38
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD13	8	0.36	0.06	0.38
(6,27)	1:33:A:SER:O	1:37:A:ILE:H	8	0.34	0.13	0.34
(6,28)	1:37:A:ILE:N	1:33:A:SER:O	8	0.28	0.11	0.29
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD11	7	2.25	0.81	2.38
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD12	7	2.25	0.81	2.38
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD13	7	2.25	0.81	2.38
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD11	7	1.41	1.08	1.11
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD12	7	1.41	1.08	1.11
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD13	7	1.41	1.08	1.11
(2,308)	2:95:B:CYS:SG	1:107:A:SER:H	7	1.2	0.42	1.03
(1,201)	1:95:A:CYS:SG	1:60:A:TYR:H	7	1.14	0.89	0.75
(5,7)	1:94:A:ILE:CB	2:97:B:GLY:CA	7	1.04	0.63	0.87
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD11	7	0.99	0.48	0.86
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD12	7	0.99	0.48	0.86
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD13	7	0.99	0.48	0.86
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD21	7	0.99	0.48	0.86
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD22	7	0.99	0.48	0.86
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD23	7	0.99	0.48	0.86
(1,199)	1:95:A:CYS:SG	1:57:A:GLY:H	7	0.97	0.8	0.58
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD11	7	0.65	0.29	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD12	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD13	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD21	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD22	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD23	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD11	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD12	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD13	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD21	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD22	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD23	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD11	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD12	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD13	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD21	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD22	7	0.65	0.29	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD23	7	0.65	0.29	0.67
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG11	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG12	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG13	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG21	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG22	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG23	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG11	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG12	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG13	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG21	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG22	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG23	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG11	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG12	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG13	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG21	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG22	7	0.35	0.41	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG23	7	0.35	0.41	0.22
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD11	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD12	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD13	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD11	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD12	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD13	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD11	7	0.24	0.07	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD12	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD13	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD11	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD12	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD13	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD11	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD12	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD13	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD11	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD12	7	0.24	0.07	0.2
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD13	7	0.24	0.07	0.2
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD11	6	2.02	0.85	2.27
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD12	6	2.02	0.85	2.27
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD13	6	2.02	0.85	2.27
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD11	6	1.94	1.12	1.83
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD12	6	1.94	1.12	1.83
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD13	6	1.94	1.12	1.83
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD11	6	1.48	0.6	1.62
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD12	6	1.48	0.6	1.62
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD13	6	1.48	0.6	1.62
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD11	6	1.41	0.69	1.58
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD12	6	1.41	0.69	1.58
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD13	6	1.41	0.69	1.58
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD11	6	1.41	0.69	1.58
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD12	6	1.41	0.69	1.58
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD13	6	1.41	0.69	1.58
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD11	6	1.41	0.69	1.58
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD12	6	1.41	0.69	1.58
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD13	6	1.41	0.69	1.58
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD11	6	1.4	0.5	1.52
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD12	6	1.4	0.5	1.52
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD13	6	1.4	0.5	1.52
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD11	6	1.4	0.5	1.52
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD12	6	1.4	0.5	1.52
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD13	6	1.4	0.5	1.52
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD11	6	1.4	0.5	1.52
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD12	6	1.4	0.5	1.52
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD13	6	1.4	0.5	1.52
(5,117)	1:66:A:VAL:CA	1:68:A:ILE:CD1	6	1.3	0.09	1.31
(2,2)	2:39:B:CYS:SG	2:1:B:MET:HA	6	1.16	0.58	1.4
(3,32)	2:71:B:ILE:HD13	3:201:A:P4P:H2D	6	1.13	0.22	1.23
(3,32)	2:71:B:ILE:HD12	3:201:A:P4P:H2B	6	1.13	0.22	1.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,32)	2:71:B:ILE:HD12	3:201:A:P4P:H2D	6	1.13	0.22	1.23
(3,32)	2:71:B:ILE:HD11	3:201:A:P4P:H2D	6	1.13	0.22	1.23
(1,219)	1:95:A:CYS:SG	1:89:A:ILE:H	6	1.12	0.8	1.14
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD11	6	0.77	0.34	0.73
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD12	6	0.77	0.34	0.73
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD13	6	0.77	0.34	0.73
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD21	6	0.77	0.34	0.73
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD22	6	0.77	0.34	0.73
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD23	6	0.77	0.34	0.73
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD11	6	0.38	0.18	0.34
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD12	6	0.38	0.18	0.34
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD13	6	0.38	0.18	0.34
(1,320)	2:39:B:CYS:SG	2:64:B:SER:H	6	0.37	0.29	0.26
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD11	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD12	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD13	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD11	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD12	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD13	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD11	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD12	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD13	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD11	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD12	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD13	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD11	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD12	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD13	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD11	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD12	6	0.3	0.12	0.31
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD13	6	0.3	0.12	0.31
(2,102)	1:41:A:CYS:SG	2:57:B:GLY:H	6	0.23	0.07	0.22
(1,177)	1:95:A:CYS:SG	1:7:A:LEU:H	5	1.16	0.86	0.98
(3,34)	1:47:A:LEU:HD12	3:201:A:P4P:H2C	5	1.08	0.66	0.79
(3,34)	1:47:A:LEU:HD12	3:201:A:P4P:H2A	5	1.08	0.66	0.79
(2,158)	2:30:B:LEU:CG	1:45:A:TRP:H	5	0.4	0.32	0.3
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD11	5	0.29	0.13	0.27
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD12	5	0.29	0.13	0.27
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD13	5	0.29	0.13	0.27
(6,29)	1:34:A:VAL:O	1:38:A:ILE:H	5	0.29	0.06	0.27
(6,30)	1:38:A:ILE:N	1:34:A:VAL:O	5	0.25	0.07	0.22
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD11	5	0.19	0.05	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD12	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD13	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD11	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD12	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD13	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD11	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD12	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD13	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD11	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD12	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD13	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD11	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD12	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD13	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD11	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD12	5	0.19	0.05	0.22
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD13	5	0.19	0.05	0.22
(2,309)	2:95:B:CYS:SG	1:110:A:HIS:H	4	0.97	0.32	0.9
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD11	4	0.56	0.34	0.53
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD12	4	0.56	0.34	0.53
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD13	4	0.56	0.34	0.53
(6,155)	2:43:B:SER:O	2:47:B:LEU:H	4	0.42	0.23	0.44
(1,351)	2:95:B:CYS:SG	2:6:B:TYR:H	4	0.4	0.11	0.44
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD11	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD12	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD13	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD11	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD12	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD13	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD11	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD12	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD13	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD11	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD12	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD13	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD11	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD12	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD13	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD11	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD12	4	0.38	0.05	0.4
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD13	4	0.38	0.05	0.4
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD11	4	0.35	0.13	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD11	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD11	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD11	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD11	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD11	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD11	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD11	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD11	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD11	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD11	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD11	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD12	4	0.35	0.13	0.32
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD13	4	0.35	0.13	0.32
(5,6)	1:90:A:GLY:CA	2:97:B:GLY:CA	4	0.33	0.18	0.29
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD11	4	0.27	0.06	0.26
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD12	4	0.27	0.06	0.26
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD13	4	0.27	0.06	0.26
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD21	4	0.27	0.06	0.26
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD22	4	0.27	0.06	0.26
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD23	4	0.27	0.06	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD11	3	1.4	0.42	1.54
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD12	3	1.4	0.42	1.54
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD13	3	1.4	0.42	1.54
(1,198)	1:95:A:CYS:SG	1:54:A:ILE:H	3	1.39	0.69	1.77
(1,218)	1:95:A:CYS:SG	1:88:A:ILE:H	3	1.18	0.01	1.18
(1,200)	1:95:A:CYS:SG	1:59:A:ALA:H	3	1.17	0.71	1.55
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD11	3	1.03	0.93	0.61
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD12	3	1.03	0.93	0.61
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD13	3	1.03	0.93	0.61
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD11	3	1.03	0.93	0.61
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD12	3	1.03	0.93	0.61
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD13	3	1.03	0.93	0.61
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD11	3	1.03	0.93	0.61
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD12	3	1.03	0.93	0.61
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD13	3	1.03	0.93	0.61
(5,1)	1:93:A:LEU:CB	2:97:B:GLY:CA	3	0.54	0.23	0.48
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD11	3	0.51	0.24	0.62
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD12	3	0.51	0.24	0.62
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD13	3	0.51	0.24	0.62
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD11	3	0.48	0.16	0.45
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD12	3	0.48	0.16	0.45
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD13	3	0.48	0.16	0.45
(3,40)	2:63:B:TRP:CE2	2:66:B:VAL:CG1	3	0.46	0.14	0.48
(3,40)	2:63:B:TRP:CE2	2:66:B:VAL:CG2	3	0.46	0.14	0.48
(6,101)	1:95:A:CYS:O	1:99:A:LEU:H	3	0.46	0.3	0.41
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD11	3	0.45	0.16	0.45
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD12	3	0.45	0.16	0.45
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD13	3	0.45	0.16	0.45
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD21	3	0.45	0.16	0.45
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD22	3	0.45	0.16	0.45
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD23	3	0.45	0.16	0.45
(6,102)	1:99:A:LEU:N	1:95:A:CYS:O	3	0.44	0.29	0.4
(2,39)	1:39:A:CYS:SG	2:62:B:ILE:H	3	0.42	0.08	0.43
(6,156)	2:47:B:LEU:N	2:43:B:SER:O	3	0.4	0.17	0.51
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD11	3	0.38	0.13	0.38
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD12	3	0.38	0.13	0.38
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD13	3	0.38	0.13	0.38
(4,1)	1:14:A:GLU:OE1	2:60:B:TYR:OH	3	0.38	0.14	0.36
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD11	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD12	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD13	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD21	3	0.36	0.06	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD22	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD23	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD11	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD12	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD13	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD21	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD22	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD23	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD11	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD12	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD13	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD21	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD22	3	0.36	0.06	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD23	3	0.36	0.06	0.33
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD11	3	0.35	0.22	0.3
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD12	3	0.35	0.22	0.3
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD13	3	0.35	0.22	0.3
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD11	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD12	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD13	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD21	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD22	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD23	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD11	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD12	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD13	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD21	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD22	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD23	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD11	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD12	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD13	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD21	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD22	3	0.35	0.05	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD23	3	0.35	0.05	0.37
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD11	3	0.34	0.08	0.36
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD12	3	0.34	0.08	0.36
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD13	3	0.34	0.08	0.36
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD11	3	0.32	0.11	0.34
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD12	3	0.32	0.11	0.34
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD13	3	0.32	0.11	0.34
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD11	3	0.32	0.14	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD12	3	0.32	0.14	0.33
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD13	3	0.32	0.14	0.33
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD21	3	0.32	0.14	0.33
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD22	3	0.32	0.14	0.33
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD23	3	0.32	0.14	0.33
(3,39)	2:63:B:TRP:CE2	2:47:B:LEU:CD1	3	0.32	0.17	0.23
(3,39)	2:63:B:TRP:CE2	2:47:B:LEU:CD2	3	0.32	0.17	0.23
(6,153)	2:42:B:ALA:O	2:46:B:LEU:H	3	0.31	0.18	0.25
(2,40)	1:39:A:CYS:SG	2:63:B:TRP:H	3	0.3	0.11	0.31
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD11	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD12	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD13	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD11	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD12	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD13	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD11	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD12	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD13	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD11	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD12	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD13	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD11	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD12	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD13	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD11	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD12	3	0.28	0.1	0.26
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD13	3	0.28	0.1	0.26
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD11	3	0.21	0.08	0.2
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD12	3	0.21	0.08	0.2
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD13	3	0.21	0.08	0.2
(1,488)	1:95:A:CYS:SG	1:54:A:ILE:HD11	2	1.97	0.07	1.97
(1,488)	1:95:A:CYS:SG	1:54:A:ILE:HD12	2	1.97	0.07	1.97
(1,488)	1:95:A:CYS:SG	1:54:A:ILE:HD13	2	1.97	0.07	1.97
(1,480)	1:95:A:CYS:SG	1:5:A:ILE:HD11	2	1.16	0.1	1.16
(1,480)	1:95:A:CYS:SG	1:5:A:ILE:HD12	2	1.16	0.1	1.16
(1,480)	1:95:A:CYS:SG	1:5:A:ILE:HD13	2	1.16	0.1	1.16
(3,26)	1:85:A:LEU:HD11	1:88:A:ILE:HD11	2	1.07	0.64	1.07
(3,26)	1:85:A:LEU:HD11	1:88:A:ILE:HD12	2	1.07	0.64	1.07
(3,26)	1:85:A:LEU:HD11	1:88:A:ILE:HD13	2	1.07	0.64	1.07
(3,26)	1:85:A:LEU:HD12	1:88:A:ILE:HD11	2	1.07	0.64	1.07
(3,26)	1:85:A:LEU:HD12	1:88:A:ILE:HD12	2	1.07	0.64	1.07
(3,26)	1:85:A:LEU:HD12	1:88:A:ILE:HD13	2	1.07	0.64	1.07

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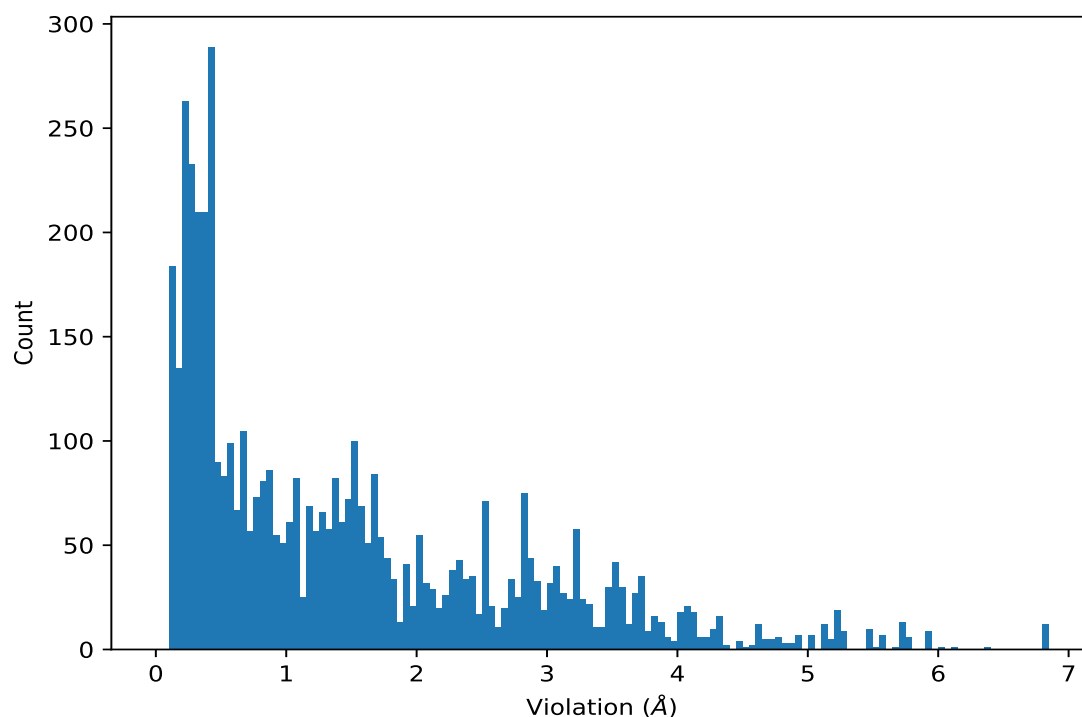
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,26)	1:85:A:LEU:HD13	1:88:A:ILE:HD11	2	1.07	0.64	1.07
(3,26)	1:85:A:LEU:HD13	1:88:A:ILE:HD12	2	1.07	0.64	1.07
(3,26)	1:85:A:LEU:HD13	1:88:A:ILE:HD13	2	1.07	0.64	1.07
(1,423)	1:5:A:ILE:CG1	1:58:A:ILE:HD11	2	0.92	0.34	0.92
(1,423)	1:5:A:ILE:CG1	1:58:A:ILE:HD12	2	0.92	0.34	0.92
(1,423)	1:5:A:ILE:CG1	1:58:A:ILE:HD13	2	0.92	0.34	0.92
(1,492)	1:95:A:CYS:SG	1:71:A:ILE:HD11	2	0.67	0.01	0.67
(1,492)	1:95:A:CYS:SG	1:71:A:ILE:HD12	2	0.67	0.01	0.67
(1,492)	1:95:A:CYS:SG	1:71:A:ILE:HD13	2	0.67	0.01	0.67
(1,182)	1:95:A:CYS:SG	1:14:A:GLU:H	2	0.63	0.04	0.63
(1,176)	1:95:A:CYS:SG	1:6:A:TYR:H	2	0.42	0.19	0.42
(3,38)	2:63:B:TRP:CD1	2:47:B:LEU:CD1	2	0.39	0.28	0.39
(3,38)	2:63:B:TRP:CD1	2:47:B:LEU:CD2	2	0.39	0.28	0.39
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD11	2	0.37	0.15	0.37
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD12	2	0.37	0.15	0.37
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD13	2	0.37	0.15	0.37
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD21	2	0.37	0.15	0.37
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD22	2	0.37	0.15	0.37
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD23	2	0.37	0.15	0.37
(3,30)	2:89:B:ILE:HD11	1:100:A:ILE:HD11	2	0.37	0.11	0.37
(3,30)	2:89:B:ILE:HD11	1:100:A:ILE:HD12	2	0.37	0.11	0.37
(3,30)	2:89:B:ILE:HD11	1:100:A:ILE:HD13	2	0.37	0.11	0.37
(3,30)	2:89:B:ILE:HD12	1:100:A:ILE:HD11	2	0.37	0.11	0.37
(3,30)	2:89:B:ILE:HD12	1:100:A:ILE:HD12	2	0.37	0.11	0.37
(3,30)	2:89:B:ILE:HD12	1:100:A:ILE:HD13	2	0.37	0.11	0.37
(3,30)	2:89:B:ILE:HD13	1:100:A:ILE:HD11	2	0.37	0.11	0.37
(3,30)	2:89:B:ILE:HD13	1:100:A:ILE:HD12	2	0.37	0.11	0.37
(3,30)	2:89:B:ILE:HD13	1:100:A:ILE:HD13	2	0.37	0.11	0.37
(1,370)	2:95:B:CYS:SG	2:43:B:SER:H	2	0.36	0.05	0.36
(1,324)	2:39:B:CYS:SG	2:68:B:ILE:H	2	0.34	0.16	0.34
(2,114)	1:41:A:CYS:SG	2:70:B:LEU:H	2	0.28	0.01	0.28
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD11	2	0.25	0.12	0.25
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD12	2	0.25	0.12	0.25
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD13	2	0.25	0.12	0.25
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD21	2	0.25	0.12	0.25
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD22	2	0.25	0.12	0.25
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD23	2	0.25	0.12	0.25
(2,421)	1:41:A:CYS:SG	2:101:B:ILE:HD11	2	0.24	0.15	0.24
(2,421)	1:41:A:CYS:SG	2:101:B:ILE:HD12	2	0.24	0.15	0.24
(2,421)	1:41:A:CYS:SG	2:101:B:ILE:HD13	2	0.24	0.15	0.24

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)
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	10	6.85
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	9	6.81
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	9	6.81
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	9	6.81
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	9	6.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	9	6.81
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	9	6.81
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	3	6.39
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	2	6.13
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	8	6.0
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	2	5.94
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	2	5.94
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	2	5.94
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	2	5.94
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	2	5.94
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	2	5.94
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	1	5.9
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	1	5.9
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	1	5.9
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	4	5.75
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	4	5.75
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	4	5.75
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	4	5.75
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	4	5.75
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	4	5.75
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	7	5.74
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	9	5.7
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	9	5.7
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	9	5.7
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	9	5.7
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	9	5.7
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	9	5.7
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	10	5.7
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	10	5.7
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	10	5.7
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	10	5.7
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	10	5.7
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	10	5.7
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	3	5.65
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	5	5.59
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	5	5.59
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	5	5.59
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	5	5.59
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	5	5.59
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	5	5.59
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	8	5.58
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	4	5.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	8	5.46
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	8	5.46
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	8	5.46
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	6	5.45
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	7	5.45
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	7	5.45
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	7	5.45
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	7	5.45
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	7	5.45
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	7	5.45
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	9	5.28
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	10	5.28
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	6	5.26
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	6	5.26
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	6	5.26
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	6	5.26
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	6	5.26
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	6	5.26
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	9	5.25
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	6	5.24
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	6	5.24
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	6	5.24
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	6	5.24
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	6	5.24
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	6	5.24
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	6	5.24
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	6	5.24
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	6	5.24
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	7	5.22
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	4	5.22
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	4	5.22
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	4	5.22
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	5	5.2
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	5	5.2
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	5	5.2
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	5	5.2
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	5	5.2
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	5	5.2
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	6	5.18
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	5	5.16
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	2	5.15
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	2	5.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	2	5.15
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	2	5.13
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	2	5.13
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	2	5.13
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	2	5.13
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	2	5.13
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	2	5.13
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	7	5.1
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	7	5.1
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	7	5.1
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	7	5.1
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	7	5.1
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	7	5.1
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	1	5.03
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	1	5.03
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	1	5.03
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	1	5.03
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	1	5.03
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	1	5.03
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	1	5.01
(2,71)	1:41:A:CYS:SG	2:2:B:ASN:H	5	4.94
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	4	4.94
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	4	4.94
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	4	4.94
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	4	4.94
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	4	4.94
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	4	4.94
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	6	4.88
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	6	4.88
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	6	4.88
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	1	4.82
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	4	4.81
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	9	4.81
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	1	4.77
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	1	4.77
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	1	4.77
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	1	4.77
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	1	4.77
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	1	4.77
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	10	4.71
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	5	4.7
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	5	4.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	5	4.7
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	8	4.7
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	8	4.68
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	8	4.68
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	8	4.68
(2,132)	1:41:A:CYS:SG	2:91:B:MET:H	2	4.67
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	10	4.65
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	3	4.62
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	3	4.62
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	3	4.62
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	3	4.62
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	3	4.62
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	3	4.62
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	3	4.61
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	3	4.61
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	3	4.61
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	3	4.61
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	3	4.61
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	3	4.61
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	6	4.58
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	4	4.57
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	2	4.5
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD11	3	4.45
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD12	3	4.45
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD13	3	4.45
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	8	4.45
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	7	4.36
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	5	4.35
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	3	4.34
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	3	4.34
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	3	4.34
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	3	4.34
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	3	4.34
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	3	4.34
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	1	4.33
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	1	4.33
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	1	4.33
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	5	4.33
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	7	4.3
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	7	4.3
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	7	4.3
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	7	4.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	7	4.3
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	7	4.3
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD11	8	4.29
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD12	8	4.29
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD13	8	4.29
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD21	8	4.29
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD22	8	4.29
(1,487)	1:95:A:CYS:SG	1:51:A:LEU:HD23	8	4.29
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	3	4.28
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	3	4.28
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	3	4.28
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	3	4.25
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	1	4.2
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	1	4.2
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	1	4.2
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	1	4.2
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	1	4.2
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	1	4.2
(2,72)	1:41:A:CYS:SG	2:4:B:TYR:H	10	4.17
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD11	3	4.15
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD12	3	4.15
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD13	3	4.15
(2,72)	1:41:A:CYS:SG	2:4:B:TYR:H	3	4.15
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	4	4.15
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	10	4.14
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	10	4.14
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	10	4.14
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	10	4.14
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	10	4.14
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	10	4.14
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD11	3	4.12
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD12	3	4.12
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD13	3	4.12
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD21	3	4.12
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD22	3	4.12
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD23	3	4.12
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	4	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	4	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	4	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	4	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	4	4.1
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	4	4.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	8	4.09
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	8	4.09
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	8	4.09
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	8	4.09
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	8	4.09
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	8	4.09
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	2	4.08
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	2	4.08
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	2	4.08
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	2	4.08
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	2	4.08
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	2	4.08
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD11	6	4.07
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD12	6	4.07
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD13	6	4.07
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	9	4.07
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	9	4.07
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	9	4.07
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	9	4.07
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	9	4.07
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	9	4.07
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	5	4.04
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	5	4.04
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	5	4.04
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	5	4.04
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	5	4.04
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	5	4.04
(2,34)	1:39:A:CYS:SG	2:56:B:THR:H	7	4.03
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD11	6	4.03
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD12	6	4.03
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD13	6	4.03
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD21	6	4.03
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD22	6	4.03
(1,465)	1:41:A:CYS:SG	1:46:A:LEU:HD23	6	4.03
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	1	4.03
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD11	7	4.0
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD12	7	4.0
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD13	7	4.0
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	3	4.0
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	7	3.99
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD11	7	3.96
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD12	7	3.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD13	7	3.96
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	6	3.94
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	9	3.91
(5,8)	2:94:B:ILE:CB	1:97:A:GLY:CA	1	3.9
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD11	3	3.9
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD12	3	3.9
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD13	3	3.9
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD11	1	3.88
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD12	1	3.88
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD13	1	3.88
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD11	1	3.88
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD12	1	3.88
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD13	1	3.88
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD11	1	3.88
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD12	1	3.88
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD13	1	3.88
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD11	8	3.86
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD12	8	3.86
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD13	8	3.86
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	9	3.85
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD11	5	3.84
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD12	5	3.84
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD13	5	3.84
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD21	5	3.84
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD22	5	3.84
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD23	5	3.84
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD11	2	3.83
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD12	2	3.83
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD13	2	3.83
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD21	2	3.83
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD22	2	3.83
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD23	2	3.83
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD11	2	3.82
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD12	2	3.82
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD13	2	3.82
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	10	3.8
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD11	10	3.79
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD12	10	3.79
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD13	10	3.79
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD11	6	3.79
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD12	6	3.79
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD13	6	3.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD21	6	3.79
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD22	6	3.79
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD23	6	3.79
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD11	10	3.73
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD12	10	3.73
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD13	10	3.73
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD11	9	3.72
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD12	9	3.72
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD13	9	3.72
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD11	8	3.72
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD12	8	3.72
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD13	8	3.72
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	4	3.72
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	4	3.72
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	4	3.72
(5,128)	1:80:A:GLY:CA	1:83:A:LEU:CG	7	3.71
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD11	4	3.71
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD12	4	3.71
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD13	4	3.71
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD21	4	3.71
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD22	4	3.71
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD23	4	3.71
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	3	3.71
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	3	3.71
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	3	3.71
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD11	6	3.7
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD12	6	3.7
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD13	6	3.7
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD21	6	3.7
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD22	6	3.7
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD23	6	3.7
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD11	10	3.7
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD12	10	3.7
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD13	10	3.7
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD21	10	3.7
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD22	10	3.7
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD23	10	3.7
(1,292)	2:39:B:CYS:SG	2:14:B:GLN:H	2	3.7
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD11	8	3.68
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD12	8	3.68
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD13	8	3.68
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD21	8	3.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD22	8	3.68
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD23	8	3.68
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD11	6	3.68
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD12	6	3.68
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD13	6	3.68
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD11	5	3.68
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD12	5	3.68
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD13	5	3.68
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD11	10	3.67
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD12	10	3.67
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD13	10	3.67
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD11	7	3.67
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD12	7	3.67
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD13	7	3.67
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD11	4	3.66
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD12	4	3.66
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD13	4	3.66
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD11	8	3.65
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD12	8	3.65
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD13	8	3.65
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD21	8	3.65
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD22	8	3.65
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD23	8	3.65
(2,72)	1:41:A:CYS:SG	2:4:B:TYR:H	4	3.64
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD11	5	3.64
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD12	5	3.64
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD13	5	3.64
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD21	5	3.64
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD22	5	3.64
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD23	5	3.64
(2,72)	1:41:A:CYS:SG	2:4:B:TYR:H	2	3.62
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	10	3.62
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	10	3.62
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	10	3.62
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	5	3.6
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	7	3.59
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	7	3.59
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	7	3.59
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD11	9	3.58
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD12	9	3.58
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD13	9	3.58
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD21	9	3.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD22	9	3.58
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD23	9	3.58
(5,128)	1:80:A:GLY:CA	1:83:A:LEU:CG	1	3.57
(5,128)	1:80:A:GLY:CA	1:83:A:LEU:CG	6	3.57
(1,291)	2:39:B:CYS:SG	2:10:B:ALA:H	6	3.57
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD11	3	3.56
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD12	3	3.56
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD13	3	3.56
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD21	3	3.56
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD22	3	3.56
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD23	3	3.56
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD11	7	3.55
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD12	7	3.55
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD13	7	3.55
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD11	7	3.55
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD12	7	3.55
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD13	7	3.55
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD11	4	3.55
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD12	4	3.55
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD13	4	3.55
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD21	4	3.55
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD22	4	3.55
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD23	4	3.55
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD11	4	3.54
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD12	4	3.54
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD13	4	3.54
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD11	9	3.54
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD12	9	3.54
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD13	9	3.54
(5,8)	2:94:B:ILE:CB	1:97:A:GLY:CA	4	3.53
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD11	3	3.53
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD12	3	3.53
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD13	3	3.53
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD21	3	3.53
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD22	3	3.53
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD23	3	3.53
(5,128)	1:80:A:GLY:CA	1:83:A:LEU:CG	3	3.52
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD11	7	3.52
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD12	7	3.52
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD13	7	3.52
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD21	7	3.52
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD22	7	3.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD23	7	3.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD11	9	3.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD12	9	3.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD13	9	3.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD21	9	3.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD22	9	3.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD23	9	3.52
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	4	3.52
(2,72)	1:41:A:CYS:SG	2:4:B:TYR:H	9	3.51
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD11	1	3.51
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD12	1	3.51
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD13	1	3.51
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD21	1	3.51
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD22	1	3.51
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD23	1	3.51
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD11	1	3.5
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD12	1	3.5
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD13	1	3.5
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD21	1	3.5
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD22	1	3.5
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD23	1	3.5
(2,72)	1:41:A:CYS:SG	2:4:B:TYR:H	8	3.5
(1,291)	2:39:B:CYS:SG	2:10:B:ALA:H	3	3.5
(5,11)	2:25:B:GLU:CD	2:22:B:LYS:CE	4	3.49
(5,8)	2:94:B:ILE:CB	1:97:A:GLY:CA	3	3.49
(5,8)	2:94:B:ILE:CB	1:97:A:GLY:CA	6	3.49
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD11	4	3.49
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD12	4	3.49
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD13	4	3.49
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD21	4	3.49
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD22	4	3.49
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD23	4	3.49
(2,72)	1:41:A:CYS:SG	2:4:B:TYR:H	5	3.48
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD11	10	3.48
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD12	10	3.48
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD13	10	3.48
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD21	10	3.48
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD22	10	3.48
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD23	10	3.48
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD11	8	3.47
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD12	8	3.47
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD13	8	3.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD11	6	3.46
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD12	6	3.46
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD13	6	3.46
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD11	9	3.46
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD12	9	3.46
(1,518)	2:5:B:ILE:CG1	2:101:B:ILE:HD13	9	3.46
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD11	4	3.46
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD12	4	3.46
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD13	4	3.46
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	7	3.46
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	6	3.46
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD11	10	3.44
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD12	10	3.44
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD13	10	3.44
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD11	1	3.42
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD12	1	3.42
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD13	1	3.42
(1,291)	2:39:B:CYS:SG	2:10:B:ALA:H	8	3.42
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	2	3.42
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD11	9	3.4
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD12	9	3.4
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD13	9	3.4
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD11	10	3.39
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD12	10	3.39
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD13	10	3.39
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD11	7	3.37
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD12	7	3.37
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD13	7	3.37
(2,34)	1:39:A:CYS:SG	2:56:B:THR:H	2	3.37
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD11	2	3.36
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD12	2	3.36
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD13	2	3.36
(5,8)	2:94:B:ILE:CB	1:97:A:GLY:CA	5	3.35
(5,128)	1:80:A:GLY:CA	1:83:A:LEU:CG	8	3.34
(5,8)	2:94:B:ILE:CB	1:97:A:GLY:CA	7	3.34
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD11	9	3.34
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD12	9	3.34
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD13	9	3.34
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD21	9	3.34
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD22	9	3.34
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD23	9	3.34
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD11	5	3.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD12	5	3.33
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD13	5	3.33
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD11	5	3.33
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD12	5	3.33
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD13	5	3.33
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD21	5	3.33
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD22	5	3.33
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD23	5	3.33
(2,34)	1:39:A:CYS:SG	2:56:B:THR:H	10	3.32
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	2	3.32
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	2	3.32
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	2	3.32
(2,72)	1:41:A:CYS:SG	2:4:B:TYR:H	6	3.3
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD11	6	3.29
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD12	6	3.29
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD13	6	3.29
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD11	1	3.29
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD12	1	3.29
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD13	1	3.29
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD11	2	3.29
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD12	2	3.29
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD13	2	3.29
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	1	3.29
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD11	8	3.28
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD12	8	3.28
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD13	8	3.28
(2,72)	1:41:A:CYS:SG	2:4:B:TYR:H	7	3.27
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD11	9	3.27
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD12	9	3.27
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD13	9	3.27
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	5	3.27
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	5	3.27
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	5	3.27
(5,8)	2:94:B:ILE:CB	1:97:A:GLY:CA	2	3.25
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD11	2	3.25
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD12	2	3.25
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD13	2	3.25
(5,128)	1:80:A:GLY:CA	1:83:A:LEU:CG	10	3.24
(2,34)	1:39:A:CYS:SG	2:56:B:THR:H	9	3.24
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	7	3.24
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	7	3.24
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	7	3.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD11	7	3.24
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD12	7	3.24
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD13	7	3.24
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD21	7	3.24
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD22	7	3.24
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD23	7	3.24
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD11	8	3.24
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD12	8	3.24
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD13	8	3.24
(1,291)	2:39:B:CYS:SG	2:10:B:ALA:H	7	3.24
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD11	8	3.23
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD12	8	3.23
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD13	8	3.23
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD11	5	3.23
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD12	5	3.23
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD13	5	3.23
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD21	5	3.23
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD22	5	3.23
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD23	5	3.23
(5,128)	1:80:A:GLY:CA	1:83:A:LEU:CG	5	3.22
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD11	1	3.22
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD12	1	3.22
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD13	1	3.22
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD11	5	3.22
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD12	5	3.22
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD13	5	3.22
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD11	6	3.21
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD12	6	3.21
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD13	6	3.21
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD21	6	3.21
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD22	6	3.21
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD23	6	3.21
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD11	4	3.21
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD12	4	3.21
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD13	4	3.21
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD21	4	3.21
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD22	4	3.21
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD23	4	3.21
(1,291)	2:39:B:CYS:SG	2:10:B:ALA:H	4	3.21
(5,8)	2:94:B:ILE:CB	1:97:A:GLY:CA	8	3.2
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD11	6	3.2
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD12	6	3.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD13	6	3.2
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD21	6	3.2
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD22	6	3.2
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD23	6	3.2
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD11	2	3.2
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD12	2	3.2
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD13	2	3.2
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD21	2	3.2
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD22	2	3.2
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD23	2	3.2
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	1	3.2
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD11	3	3.19
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD12	3	3.19
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD13	3	3.19
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD11	1	3.19
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD12	1	3.19
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD13	1	3.19
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD11	5	3.18
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD12	5	3.18
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD13	5	3.18
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD21	5	3.18
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD22	5	3.18
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD23	5	3.18
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD11	5	3.16
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD12	5	3.16
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD13	5	3.16
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	9	3.16
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	9	3.16
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	9	3.16
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD11	8	3.16
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD12	8	3.16
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD13	8	3.16
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD21	8	3.16
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD22	8	3.16
(1,494)	1:95:A:CYS:SG	1:74:A:LEU:HD23	8	3.16
(2,35)	1:39:A:CYS:SG	2:57:B:GLY:H	7	3.14
(1,180)	1:95:A:CYS:SG	1:10:A:ALA:H	10	3.14
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD11	10	3.13
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD12	10	3.13
(1,528)	2:39:B:CYS:SG	2:68:B:ILE:HD13	10	3.13
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD11	3	3.12
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD12	3	3.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD13	3	3.12
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD21	3	3.12
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD22	3	3.12
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD23	3	3.12
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD11	1	3.11
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD12	1	3.11
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD13	1	3.11
(2,38)	1:39:A:CYS:SG	2:60:B:TYR:H	2	3.11
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD11	8	3.11
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD12	8	3.11
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD13	8	3.11
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD21	8	3.11
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD22	8	3.11
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD23	8	3.11
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD11	9	3.1
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD12	9	3.1
(2,450)	2:41:B:CYS:SG	1:71:A:ILE:HD13	9	3.1
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD11	5	3.1
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD12	5	3.1
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD13	5	3.1
(5,63)	1:25:A:GLU:CD	1:22:A:LYS:CE	6	3.09
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD11	4	3.08
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD12	4	3.08
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD13	4	3.08
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD11	7	3.07
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD12	7	3.07
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD13	7	3.07
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD11	7	3.07
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD12	7	3.07
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD13	7	3.07
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD11	7	3.07
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD12	7	3.07
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD13	7	3.07
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD11	9	3.07
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD12	9	3.07
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD13	9	3.07
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD21	9	3.07
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD22	9	3.07
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD23	9	3.07
(2,38)	1:39:A:CYS:SG	2:60:B:TYR:H	7	3.07
(2,34)	1:39:A:CYS:SG	2:56:B:THR:H	6	3.07
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD11	5	3.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD12	5	3.07
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD13	5	3.07
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD11	10	3.06
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD12	10	3.06
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD13	10	3.06
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD21	10	3.06
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD22	10	3.06
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD23	10	3.06
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD11	10	3.06
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD12	10	3.06
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD13	10	3.06
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD11	10	3.06
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD12	10	3.06
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD13	10	3.06
(2,29)	1:39:A:CYS:SG	2:49:B:GLN:H	7	3.06
(5,128)	1:80:A:GLY:CA	1:83:A:LEU:CG	9	3.05
(5,63)	1:25:A:GLU:CD	1:22:A:LYS:CE	7	3.05
(1,291)	2:39:B:CYS:SG	2:10:B:ALA:H	9	3.05
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD11	1	3.04
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD12	1	3.04
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD13	1	3.04
(5,128)	1:80:A:GLY:CA	1:83:A:LEU:CG	2	3.03
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD11	1	3.03
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD12	1	3.03
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD13	1	3.03
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD21	1	3.03
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD22	1	3.03
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD23	1	3.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD11	7	3.0
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD12	7	3.0
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD13	7	3.0
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD21	7	3.0
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD22	7	3.0
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD23	7	3.0
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD11	7	3.0
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD12	7	3.0
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD13	7	3.0
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD21	7	3.0
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD22	7	3.0
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD23	7	3.0
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD11	7	3.0
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD12	7	3.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD13	7	3.0
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD21	7	3.0
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD22	7	3.0
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD23	7	3.0
(2,38)	1:39:A:CYS:SG	2:60:B:TYR:H	10	3.0
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD11	4	3.0
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD12	4	3.0
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD13	4	3.0
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD11	8	2.98
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD12	8	2.98
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD13	8	2.98
(5,11)	2:25:B:GLU:CD	2:22:B:LYS:CE	2	2.97
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD11	2	2.97
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD12	2	2.97
(1,535)	2:39:B:CYS:SG	2:94:B:ILE:HD13	2	2.97
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD11	10	2.95
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD12	10	2.95
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD13	10	2.95
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD21	10	2.95
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD22	10	2.95
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD23	10	2.95
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD11	4	2.95
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD12	4	2.95
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD13	4	2.95
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD21	4	2.95
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD22	4	2.95
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD23	4	2.95
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD11	1	2.94
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD12	1	2.94
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD13	1	2.94
(1,180)	1:95:A:CYS:SG	1:10:A:ALA:H	9	2.94
(2,34)	1:39:A:CYS:SG	2:56:B:THR:H	8	2.93
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD11	4	2.92
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD12	4	2.92
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD13	4	2.92
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD11	9	2.91
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD12	9	2.91
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD13	9	2.91
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD11	9	2.91
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD12	9	2.91
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD13	9	2.91
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD11	9	2.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD12	9	2.91
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD13	9	2.91
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD11	9	2.91
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD12	9	2.91
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD13	9	2.91
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD11	9	2.91
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD12	9	2.91
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD13	9	2.91
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD11	9	2.91
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD12	9	2.91
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD13	9	2.91
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD11	1	2.91
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD12	1	2.91
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD13	1	2.91
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD21	1	2.91
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD22	1	2.91
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD23	1	2.91
(1,291)	2:39:B:CYS:SG	2:10:B:ALA:H	5	2.91
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD11	2	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD12	2	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD13	2	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD21	2	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD22	2	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD23	2	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD11	6	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD12	6	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD13	6	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD21	6	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD22	6	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD23	6	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD11	9	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD12	9	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD13	9	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD21	9	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD22	9	2.89
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD23	9	2.89
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD11	6	2.88
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD12	6	2.88
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD13	6	2.88
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD21	6	2.88
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD22	6	2.88
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD23	6	2.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,8)	2:94:B:ILE:CB	1:97:A:GLY:CA	9	2.87
(5,63)	1:25:A:GLU:CD	1:22:A:LYS:CE	8	2.86
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD11	2	2.86
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD12	2	2.86
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD13	2	2.86
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD21	2	2.86
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD22	2	2.86
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD23	2	2.86
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD11	8	2.86
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD12	8	2.86
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD13	8	2.86
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD21	8	2.86
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD22	8	2.86
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD23	8	2.86
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD11	9	2.85
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD12	9	2.85
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD13	9	2.85
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD21	9	2.85
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD22	9	2.85
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD23	9	2.85
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD11	1	2.84
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD12	1	2.84
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD13	1	2.84
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD21	1	2.84
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD22	1	2.84
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD23	1	2.84
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD11	7	2.84
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD12	7	2.84
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD13	7	2.84
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD21	7	2.84
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD22	7	2.84
(1,452)	1:39:A:CYS:SG	1:83:A:LEU:HD23	7	2.84
(2,72)	1:41:A:CYS:SG	2:4:B:TYR:H	1	2.83
(5,11)	2:25:B:GLU:CD	2:22:B:LYS:CE	5	2.82
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD11	10	2.82
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD12	10	2.82
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD13	10	2.82
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD11	7	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD12	7	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD13	7	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD21	7	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD22	7	2.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD23	7	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD11	8	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD12	8	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD13	8	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD21	8	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD22	8	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD23	8	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD11	10	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD12	10	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD13	10	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD21	10	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD22	10	2.81
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD23	10	2.81
(1,179)	1:95:A:CYS:SG	1:9:A:GLY:H	10	2.81
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD11	1	2.8
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD12	1	2.8
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD13	1	2.8
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD11	1	2.8
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD12	1	2.8
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD13	1	2.8
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD11	1	2.8
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD12	1	2.8
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD13	1	2.8
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD11	1	2.8
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD12	1	2.8
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD13	1	2.8
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD11	1	2.8
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD12	1	2.8
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD13	1	2.8
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD11	1	2.8
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD12	1	2.8
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD13	1	2.8
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD11	10	2.8
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD12	10	2.8
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD13	10	2.8
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD11	10	2.8
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD12	10	2.8
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD13	10	2.8
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD11	10	2.8
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD12	10	2.8
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD13	10	2.8
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD11	10	2.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD12	10	2.8
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD13	10	2.8
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD11	10	2.8
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD12	10	2.8
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD13	10	2.8
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD11	10	2.8
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD12	10	2.8
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD13	10	2.8
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD11	2	2.8
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD12	2	2.8
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD13	2	2.8
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD11	3	2.79
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD12	3	2.79
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD13	3	2.79
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD21	3	2.79
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD22	3	2.79
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD23	3	2.79
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD11	7	2.79
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD12	7	2.79
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD13	7	2.79
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD21	7	2.79
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD22	7	2.79
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD23	7	2.79
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD11	2	2.77
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD12	2	2.77
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD13	2	2.77
(5,8)	2:94:B:ILE:CB	1:97:A:GLY:CA	10	2.76
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD11	8	2.75
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD12	8	2.75
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD13	8	2.75
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD11	6	2.75
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD12	6	2.75
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD13	6	2.75
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD21	6	2.75
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD22	6	2.75
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD23	6	2.75
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD11	8	2.74
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD12	8	2.74
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD13	8	2.74
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD21	8	2.74
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD22	8	2.74
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD23	8	2.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD11	10	2.74
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD12	10	2.74
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD13	10	2.74
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD21	10	2.74
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD22	10	2.74
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD23	10	2.74
(5,63)	1:25:A:GLU:CD	1:22:A:LYS:CE	2	2.73
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD11	6	2.73
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD12	6	2.73
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD13	6	2.73
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD11	3	2.73
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD12	3	2.73
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD13	3	2.73
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD21	3	2.73
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD22	3	2.73
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD23	3	2.73
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD11	7	2.72
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD12	7	2.72
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD13	7	2.72
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD11	8	2.72
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD12	8	2.72
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD13	8	2.72
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD21	8	2.72
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD22	8	2.72
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD23	8	2.72
(5,128)	1:80:A:GLY:CA	1:83:A:LEU:CG	4	2.71
(2,34)	1:39:A:CYS:SG	2:56:B:THR:H	1	2.71
(2,34)	1:39:A:CYS:SG	2:56:B:THR:H	4	2.71
(5,63)	1:25:A:GLU:CD	1:22:A:LYS:CE	10	2.69
(1,291)	2:39:B:CYS:SG	2:10:B:ALA:H	1	2.69
(1,300)	2:39:B:CYS:SG	2:28:B:THR:H	1	2.68
(1,291)	2:39:B:CYS:SG	2:10:B:ALA:H	10	2.67
(1,167)	1:41:A:CYS:SG	1:97:A:GLY:H	10	2.67
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD11	5	2.66
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD12	5	2.66
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD13	5	2.66
(2,34)	1:39:A:CYS:SG	2:56:B:THR:H	3	2.66
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD11	8	2.65
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD12	8	2.65
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD13	8	2.65
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD11	6	2.65
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD12	6	2.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD13	6	2.65
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD21	6	2.65
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD22	6	2.65
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD23	6	2.65
(1,291)	2:39:B:CYS:SG	2:10:B:ALA:H	2	2.65
(1,179)	1:95:A:CYS:SG	1:9:A:GLY:H	9	2.65
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD11	2	2.63
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD12	2	2.63
(2,417)	1:41:A:CYS:SG	2:89:B:ILE:HD13	2	2.63
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	3	2.63
(5,63)	1:25:A:GLU:CD	1:22:A:LYS:CE	4	2.62
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD11	3	2.62
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD12	3	2.62
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD13	3	2.62
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD21	3	2.62
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD22	3	2.62
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD23	3	2.62
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD11	5	2.58
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD12	5	2.58
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD13	5	2.58
(1,201)	1:95:A:CYS:SG	1:60:A:TYR:H	10	2.57
(2,35)	1:39:A:CYS:SG	2:57:B:GLY:H	2	2.56
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD11	6	2.56
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD12	6	2.56
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD13	6	2.56
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD11	1	2.56
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD12	1	2.56
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD13	1	2.56
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD21	1	2.56
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD22	1	2.56
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD23	1	2.56
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD11	4	2.55
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD12	4	2.55
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD13	4	2.55
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD11	4	2.55
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD12	4	2.55
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD13	4	2.55
(1,97)	1:39:A:CYS:SG	1:75:A:SER:H	6	2.55
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD11	6	2.54
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD12	6	2.54
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD13	6	2.54
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD11	6	2.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD12	6	2.54
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD13	6	2.54
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD11	6	2.54
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD12	6	2.54
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD13	6	2.54
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD11	8	2.54
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD12	8	2.54
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD13	8	2.54
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD11	8	2.54
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD12	8	2.54
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD13	8	2.54
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD11	8	2.54
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD12	8	2.54
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD13	8	2.54
(2,34)	1:39:A:CYS:SG	2:56:B:THR:H	5	2.54
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD11	7	2.54
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD12	7	2.54
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD13	7	2.54
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD21	7	2.54
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD22	7	2.54
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD23	7	2.54
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD11	7	2.54
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD12	7	2.54
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD13	7	2.54
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD21	7	2.54
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD22	7	2.54
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD23	7	2.54
(2,36)	1:39:A:CYS:SG	2:58:B:ILE:H	7	2.53
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD11	4	2.53
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD12	4	2.53
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD13	4	2.53
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD21	4	2.53
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD22	4	2.53
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD23	4	2.53
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD11	3	2.52
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD12	3	2.52
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD13	3	2.52
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD21	3	2.52
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD22	3	2.52
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD23	3	2.52
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD11	1	2.52
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD12	1	2.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD13	1	2.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD11	2	2.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD12	2	2.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD13	2	2.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD21	2	2.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD22	2	2.52
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD23	2	2.52
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD11	9	2.52
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD12	9	2.52
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD13	9	2.52
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD11	7	2.51
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD12	7	2.51
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD13	7	2.51
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD11	2	2.5
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD12	2	2.5
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD13	2	2.5
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD21	2	2.5
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD22	2	2.5
(2,428)	2:39:B:CYS:SG	1:51:A:LEU:HD23	2	2.5
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD11	10	2.5
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD12	10	2.5
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD13	10	2.5
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD21	10	2.5
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD22	10	2.5
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD23	10	2.5
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD11	5	2.49
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD12	5	2.49
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD13	5	2.49
(1,220)	1:95:A:CYS:SG	1:90:A:GLY:H	5	2.49
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD11	4	2.48
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD12	4	2.48
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD13	4	2.48
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD21	4	2.48
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD22	4	2.48
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD23	4	2.48
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD11	5	2.47
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD12	5	2.47
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD13	5	2.47
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD21	5	2.47
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD22	5	2.47
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD23	5	2.47
(1,201)	1:95:A:CYS:SG	1:60:A:TYR:H	9	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:39:A:CYS:SG	2:57:B:GLY:H	10	2.43
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD11	2	2.43
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD12	2	2.43
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD13	2	2.43
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD21	2	2.43
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD22	2	2.43
(1,523)	2:39:B:CYS:SG	2:46:B:LEU:HD23	2	2.43
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD11	5	2.42
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD12	5	2.42
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD13	5	2.42
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD21	5	2.42
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD22	5	2.42
(1,522)	2:39:B:CYS:SG	2:30:B:LEU:HD23	5	2.42
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD11	6	2.42
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD12	6	2.42
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD13	6	2.42
(1,300)	2:39:B:CYS:SG	2:28:B:THR:H	4	2.42
(1,220)	1:95:A:CYS:SG	1:90:A:GLY:H	2	2.42
(1,97)	1:39:A:CYS:SG	1:75:A:SER:H	7	2.42
(2,38)	1:39:A:CYS:SG	2:60:B:TYR:H	9	2.41
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD11	2	2.41
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD12	2	2.41
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD13	2	2.41
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD11	2	2.41
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD12	2	2.41
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD13	2	2.41
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD21	2	2.41
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD22	2	2.41
(1,421)	1:5:A:ILE:CG1	1:51:A:LEU:HD23	2	2.41
(1,220)	1:95:A:CYS:SG	1:90:A:GLY:H	4	2.41
(2,38)	1:39:A:CYS:SG	2:60:B:TYR:H	3	2.4
(2,38)	1:39:A:CYS:SG	2:60:B:TYR:H	6	2.4
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD11	4	2.4
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD12	4	2.4
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD13	4	2.4
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD11	8	2.38
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD12	8	2.38
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD13	8	2.38
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD11	1	2.38
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD12	1	2.38
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD13	1	2.38
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD11	9	2.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD12	9	2.37
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD13	9	2.37
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD11	4	2.37
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD12	4	2.37
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD13	4	2.37
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD21	4	2.37
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD22	4	2.37
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD23	4	2.37
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD11	9	2.36
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD12	9	2.36
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD13	9	2.36
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD21	9	2.36
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD22	9	2.36
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD23	9	2.36
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD11	9	2.36
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD12	9	2.36
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD13	9	2.36
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD21	9	2.36
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD22	9	2.36
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD23	9	2.36
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD11	9	2.36
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD12	9	2.36
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD13	9	2.36
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD21	9	2.36
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD22	9	2.36
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD23	9	2.36
(2,38)	1:39:A:CYS:SG	2:60:B:TYR:H	4	2.35
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD11	9	2.34
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD12	9	2.34
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD13	9	2.34
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD21	9	2.34
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD22	9	2.34
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD23	9	2.34
(1,199)	1:95:A:CYS:SG	1:57:A:GLY:H	10	2.33
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD1	5	2.32
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD2	5	2.32
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD11	9	2.32
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD12	9	2.32
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD13	9	2.32
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD11	9	2.32
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD12	9	2.32
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD13	9	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD11	9	2.32
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD12	9	2.32
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD13	9	2.32
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD11	5	2.32
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD12	5	2.32
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD13	5	2.32
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD11	3	2.32
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD12	3	2.32
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD13	3	2.32
(5,63)	1:25:A:GLU:CD	1:22:A:LYS:CE	5	2.31
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD11	3	2.31
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD12	3	2.31
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD13	3	2.31
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD11	3	2.31
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD12	3	2.31
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD13	3	2.31
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD11	3	2.31
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD12	3	2.31
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD13	3	2.31
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD11	3	2.31
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD12	3	2.31
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD13	3	2.31
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD11	3	2.31
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD12	3	2.31
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD13	3	2.31
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD11	3	2.31
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD12	3	2.31
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD13	3	2.31
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD11	10	2.29
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD12	10	2.29
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD13	10	2.29
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD21	10	2.29
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD22	10	2.29
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD23	10	2.29
(2,36)	1:39:A:CYS:SG	2:58:B:ILE:H	2	2.29
(2,35)	1:39:A:CYS:SG	2:57:B:GLY:H	6	2.29
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD11	8	2.29
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD12	8	2.29
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD13	8	2.29
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD21	8	2.29
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD22	8	2.29
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD23	8	2.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD11	1	2.28
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD12	1	2.28
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD13	1	2.28
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD11	1	2.28
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD12	1	2.28
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD13	1	2.28
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD11	1	2.28
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD12	1	2.28
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD13	1	2.28
(1,177)	1:95:A:CYS:SG	1:7:A:LEU:H	10	2.28
(3,33)	1:47:A:LEU:HD11	3:201:A:P4P:H2C	9	2.27
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD11	2	2.27
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD12	2	2.27
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD13	2	2.27
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD1	8	2.26
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD2	8	2.26
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD1	10	2.26
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD2	10	2.26
(3,33)	1:47:A:LEU:HD11	3:201:A:P4P:H2C	4	2.26
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD11	10	2.26
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD12	10	2.26
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD13	10	2.26
(5,11)	2:25:B:GLU:CD	2:22:B:LYS:CE	1	2.25
(5,7)	1:94:A:ILE:CB	2:97:B:GLY:CA	1	2.25
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD11	7	2.24
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD12	7	2.24
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD13	7	2.24
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD21	7	2.24
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD22	7	2.24
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD23	7	2.24
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD11	3	2.23
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD12	3	2.23
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD13	3	2.23
(1,304)	2:39:B:CYS:SG	2:33:B:SER:H	1	2.23
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD11	1	2.22
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD12	1	2.22
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD13	1	2.22
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD11	5	2.2
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD12	5	2.2
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD13	5	2.2
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD11	5	2.2
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD12	5	2.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD13	5	2.2
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD11	5	2.2
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD12	5	2.2
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD13	5	2.2
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD11	3	2.2
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD12	3	2.2
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD13	3	2.2
(1,300)	2:39:B:CYS:SG	2:28:B:THR:H	3	2.2
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD11	3	2.18
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD12	3	2.18
(2,392)	1:39:A:CYS:SG	2:37:B:ILE:HD13	3	2.18
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD11	6	2.17
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD12	6	2.17
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD13	6	2.17
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD21	6	2.17
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD22	6	2.17
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD23	6	2.17
(2,29)	1:39:A:CYS:SG	2:49:B:GLN:H	3	2.17
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD11	1	2.16
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD12	1	2.16
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD13	1	2.16
(1,304)	2:39:B:CYS:SG	2:33:B:SER:H	4	2.16
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD11	1	2.15
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD12	1	2.15
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD13	1	2.15
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD21	1	2.15
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD22	1	2.15
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD23	1	2.15
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD1	7	2.14
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD2	7	2.14
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD11	9	2.14
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD12	9	2.14
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD13	9	2.14
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD11	9	2.14
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD12	9	2.14
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD13	9	2.14
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD11	9	2.14
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD12	9	2.14
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD13	9	2.14
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD11	4	2.13
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD12	4	2.13
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD13	4	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD11	6	2.11
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD12	6	2.11
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD13	6	2.11
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD11	5	2.11
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD12	5	2.11
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD13	5	2.11
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD21	5	2.11
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD22	5	2.11
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD23	5	2.11
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD11	5	2.1
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD12	5	2.1
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD13	5	2.1
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD21	5	2.1
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD22	5	2.1
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD23	5	2.1
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD11	7	2.09
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD12	7	2.09
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD13	7	2.09
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD11	7	2.09
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD12	7	2.09
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD13	7	2.09
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD11	7	2.09
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD12	7	2.09
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD13	7	2.09
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD11	7	2.09
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD12	7	2.09
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD13	7	2.09
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD11	7	2.09
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD12	7	2.09
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD13	7	2.09
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD11	7	2.09
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD12	7	2.09
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD13	7	2.09
(1,199)	1:95:A:CYS:SG	1:57:A:GLY:H	9	2.08
(1,97)	1:39:A:CYS:SG	1:75:A:SER:H	3	2.08
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD1	6	2.07
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD2	6	2.07
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD11	4	2.07
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD12	4	2.07
(2,427)	2:39:B:CYS:SG	1:37:A:ILE:HD13	4	2.07
(2,35)	1:39:A:CYS:SG	2:57:B:GLY:H	9	2.07
(1,25)	1:5:A:ILE:CG1	1:54:A:ILE:H	8	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,36)	1:39:A:CYS:SG	2:58:B:ILE:H	10	2.06
(2,30)	1:39:A:CYS:SG	2:51:B:LEU:H	7	2.05
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD11	3	2.05
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD12	3	2.05
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD13	3	2.05
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD11	2	2.04
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD12	2	2.04
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD13	2	2.04
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD11	7	2.04
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD12	7	2.04
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD13	7	2.04
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD21	7	2.04
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD22	7	2.04
(1,495)	1:95:A:CYS:SG	1:83:A:LEU:HD23	7	2.04
(1,488)	1:95:A:CYS:SG	1:54:A:ILE:HD11	10	2.04
(1,488)	1:95:A:CYS:SG	1:54:A:ILE:HD12	10	2.04
(1,488)	1:95:A:CYS:SG	1:54:A:ILE:HD13	10	2.04
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD11	1	2.04
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD12	1	2.04
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD13	1	2.04
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD21	1	2.04
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD22	1	2.04
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD23	1	2.04
(1,304)	2:39:B:CYS:SG	2:33:B:SER:H	3	2.04
(1,300)	2:39:B:CYS:SG	2:28:B:THR:H	6	2.04
(5,63)	1:25:A:GLU:CD	1:22:A:LYS:CE	3	2.03
(2,38)	1:39:A:CYS:SG	2:60:B:TYR:H	5	2.03
(2,38)	1:39:A:CYS:SG	2:60:B:TYR:H	1	2.02
(2,35)	1:39:A:CYS:SG	2:57:B:GLY:H	1	2.02
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD11	6	2.02
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD12	6	2.02
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD13	6	2.02
(1,219)	1:95:A:CYS:SG	1:89:A:ILE:H	5	2.02
(1,177)	1:95:A:CYS:SG	1:7:A:LEU:H	9	2.02
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD1	9	2.01
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD2	9	2.01
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD11	2	2.01
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD12	2	2.01
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD13	2	2.01
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD11	2	2.01
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD12	2	2.01
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD13	2	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD11	2	2.01
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD12	2	2.01
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD13	2	2.01
(2,36)	1:39:A:CYS:SG	2:58:B:ILE:H	6	2.01
(1,300)	2:39:B:CYS:SG	2:28:B:THR:H	7	2.01
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD11	10	2.0
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD12	10	2.0
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD13	10	2.0
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD11	10	2.0
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD12	10	2.0
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD13	10	2.0
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD11	10	2.0
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD12	10	2.0
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD13	10	2.0
(2,308)	2:95:B:CYS:SG	1:107:A:SER:H	7	2.0
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD11	7	2.0
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD12	7	2.0
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD13	7	2.0
(3,34)	1:47:A:LEU:HD12	3:201:A:P4P:H2A	10	1.99
(1,198)	1:95:A:CYS:SG	1:54:A:ILE:H	10	1.99
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD11	5	1.97
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD12	5	1.97
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD13	5	1.97
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD11	5	1.97
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD12	5	1.97
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD13	5	1.97
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD11	5	1.97
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD12	5	1.97
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD13	5	1.97
(1,97)	1:39:A:CYS:SG	1:75:A:SER:H	8	1.96
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD1	2	1.95
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD2	2	1.95
(2,2)	2:39:B:CYS:SG	2:1:B:MET:HA	10	1.95
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD11	1	1.95
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD12	1	1.95
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD13	1	1.95
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD21	1	1.95
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD22	1	1.95
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD23	1	1.95
(5,63)	1:25:A:GLU:CD	1:22:A:LYS:CE	1	1.94
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD11	1	1.94
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD12	1	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD13	1	1.94
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD11	10	1.94
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD12	10	1.94
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD13	10	1.94
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD11	2	1.94
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD12	2	1.94
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD13	2	1.94
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD21	2	1.94
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD22	2	1.94
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD23	2	1.94
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD11	2	1.94
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD12	2	1.94
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD13	2	1.94
(1,304)	2:39:B:CYS:SG	2:33:B:SER:H	2	1.94
(1,97)	1:39:A:CYS:SG	1:75:A:SER:H	10	1.94
(1,25)	1:5:A:ILE:CG1	1:54:A:ILE:H	7	1.94
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD11	9	1.93
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD12	9	1.93
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD13	9	1.93
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD21	9	1.93
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD22	9	1.93
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD23	9	1.93
(1,304)	2:39:B:CYS:SG	2:33:B:SER:H	6	1.93
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD11	1	1.92
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD12	1	1.92
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD13	1	1.92
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD21	1	1.92
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD22	1	1.92
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD23	1	1.92
(5,40)	2:63:B:TRP:CE2	2:62:B:ILE:CG2	9	1.91
(2,35)	1:39:A:CYS:SG	2:57:B:GLY:H	3	1.91
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD11	5	1.9
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD12	5	1.9
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD13	5	1.9
(1,488)	1:95:A:CYS:SG	1:54:A:ILE:HD11	9	1.9
(1,488)	1:95:A:CYS:SG	1:54:A:ILE:HD12	9	1.9
(1,488)	1:95:A:CYS:SG	1:54:A:ILE:HD13	9	1.9
(1,219)	1:95:A:CYS:SG	1:89:A:ILE:H	4	1.9
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD11	7	1.89
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD12	7	1.89
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD13	7	1.89
(1,304)	2:39:B:CYS:SG	2:33:B:SER:H	7	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD11	1	1.86
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD12	1	1.86
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD13	1	1.86
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD21	1	1.86
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD22	1	1.86
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD23	1	1.86
(1,304)	2:39:B:CYS:SG	2:33:B:SER:H	5	1.86
(2,35)	1:39:A:CYS:SG	2:57:B:GLY:H	5	1.85
(2,35)	1:39:A:CYS:SG	2:57:B:GLY:H	8	1.85
(5,63)	1:25:A:GLU:CD	1:22:A:LYS:CE	9	1.84
(5,40)	2:63:B:TRP:CE2	2:62:B:ILE:CG2	10	1.84
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD11	3	1.84
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD12	3	1.84
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD13	3	1.84
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD11	7	1.83
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD12	7	1.83
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD13	7	1.83
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD21	7	1.83
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD22	7	1.83
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD23	7	1.83
(1,97)	1:39:A:CYS:SG	1:75:A:SER:H	9	1.83
(1,296)	2:39:B:CYS:SG	2:24:B:SER:H	1	1.82
(1,219)	1:95:A:CYS:SG	1:89:A:ILE:H	2	1.82
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD11	6	1.81
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD12	6	1.81
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD13	6	1.81
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD21	6	1.81
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD22	6	1.81
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD23	6	1.81
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD11	5	1.81
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD12	5	1.81
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD13	5	1.81
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD11	9	1.81
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD12	9	1.81
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD13	9	1.81
(1,304)	2:39:B:CYS:SG	2:33:B:SER:H	10	1.81
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD11	5	1.8
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD12	5	1.8
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD13	5	1.8
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD21	5	1.8
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD22	5	1.8
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD23	5	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:39:A:CYS:SG	2:60:B:TYR:H	8	1.8
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD1	4	1.79
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD2	4	1.79
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD11	3	1.79
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD12	3	1.79
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD13	3	1.79
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD11	3	1.79
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD12	3	1.79
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD13	3	1.79
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD11	3	1.79
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD12	3	1.79
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD13	3	1.79
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD11	6	1.79
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD12	6	1.79
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD13	6	1.79
(1,200)	1:95:A:CYS:SG	1:59:A:ALA:H	10	1.79
(1,180)	1:95:A:CYS:SG	1:10:A:ALA:H	6	1.79
(1,304)	2:39:B:CYS:SG	2:33:B:SER:H	8	1.78
(5,40)	2:63:B:TRP:CE2	2:62:B:ILE:CG2	7	1.77
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD11	2	1.77
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD12	2	1.77
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD13	2	1.77
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD21	2	1.77
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD22	2	1.77
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD23	2	1.77
(1,304)	2:39:B:CYS:SG	2:33:B:SER:H	9	1.77
(1,198)	1:95:A:CYS:SG	1:54:A:ILE:H	9	1.77
(5,11)	2:25:B:GLU:CD	2:22:B:LYS:CE	7	1.76
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD11	3	1.76
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD12	3	1.76
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD13	3	1.76
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD11	9	1.76
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD12	9	1.76
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD13	9	1.76
(1,296)	2:39:B:CYS:SG	2:24:B:SER:H	7	1.76
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD11	8	1.75
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD12	8	1.75
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD13	8	1.75
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD21	8	1.75
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD22	8	1.75
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD23	8	1.75
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD11	3	1.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD12	3	1.75
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD13	3	1.75
(1,180)	1:95:A:CYS:SG	1:10:A:ALA:H	7	1.75
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD11	6	1.74
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD12	6	1.74
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD13	6	1.74
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD11	6	1.74
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD12	6	1.74
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD13	6	1.74
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD11	6	1.74
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD12	6	1.74
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD13	6	1.74
(1,300)	2:39:B:CYS:SG	2:28:B:THR:H	5	1.74
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD1	1	1.73
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD2	1	1.73
(2,29)	1:39:A:CYS:SG	2:49:B:GLN:H	5	1.73
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD11	3	1.72
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD12	3	1.72
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD13	3	1.72
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD11	3	1.72
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD12	3	1.72
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD13	3	1.72
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD11	3	1.72
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD12	3	1.72
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD13	3	1.72
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD11	10	1.72
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD12	10	1.72
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD13	10	1.72
(2,29)	1:39:A:CYS:SG	2:49:B:GLN:H	6	1.72
(3,26)	1:85:A:LEU:HD11	1:88:A:ILE:HD11	10	1.71
(3,26)	1:85:A:LEU:HD11	1:88:A:ILE:HD12	10	1.71
(3,26)	1:85:A:LEU:HD11	1:88:A:ILE:HD13	10	1.71
(3,26)	1:85:A:LEU:HD12	1:88:A:ILE:HD11	10	1.71
(3,26)	1:85:A:LEU:HD12	1:88:A:ILE:HD12	10	1.71
(3,26)	1:85:A:LEU:HD12	1:88:A:ILE:HD13	10	1.71
(3,26)	1:85:A:LEU:HD13	1:88:A:ILE:HD11	10	1.71
(3,26)	1:85:A:LEU:HD13	1:88:A:ILE:HD12	10	1.71
(3,26)	1:85:A:LEU:HD13	1:88:A:ILE:HD13	10	1.71
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD11	10	1.71
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD12	10	1.71
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD13	10	1.71
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD21	10	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD22	10	1.71
(1,520)	2:39:B:CYS:SG	2:7:B:LEU:HD23	10	1.71
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD11	7	1.7
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD12	7	1.7
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD13	7	1.7
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD21	7	1.7
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD22	7	1.7
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD23	7	1.7
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD11	8	1.7
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD12	8	1.7
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD13	8	1.7
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD21	8	1.7
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD22	8	1.7
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD23	8	1.7
(1,179)	1:95:A:CYS:SG	1:9:A:GLY:H	6	1.7
(3,34)	1:47:A:LEU:HD12	3:201:A:P4P:H2C	2	1.69
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD11	3	1.69
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD12	3	1.69
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD13	3	1.69
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD21	3	1.69
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD22	3	1.69
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD23	3	1.69
(1,25)	1:5:A:ILE:CG1	1:54:A:ILE:H	10	1.69
(5,40)	2:63:B:TRP:CE2	2:62:B:ILE:CG2	5	1.68
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD11	2	1.68
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD12	2	1.68
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD13	2	1.68
(2,75)	1:41:A:CYS:SG	2:8:B:GLY:H	3	1.68
(2,37)	1:39:A:CYS:SG	2:59:B:ALA:H	7	1.68
(2,36)	1:39:A:CYS:SG	2:58:B:ILE:H	9	1.68
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD11	3	1.68
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD12	3	1.68
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD13	3	1.68
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD11	5	1.68
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD12	5	1.68
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD13	5	1.68
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD11	6	1.67
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD12	6	1.67
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD13	6	1.67
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD11	9	1.67
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD12	9	1.67
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD13	9	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD11	4	1.67
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD12	4	1.67
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD13	4	1.67
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD11	10	1.66
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD12	10	1.66
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD13	10	1.66
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD21	10	1.66
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD22	10	1.66
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD23	10	1.66
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD11	1	1.66
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD12	1	1.66
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD13	1	1.66
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD11	2	1.65
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD12	2	1.65
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD13	2	1.65
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD11	2	1.65
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD12	2	1.65
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD13	2	1.65
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD11	2	1.65
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD12	2	1.65
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD13	2	1.65
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD11	2	1.65
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD12	2	1.65
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD13	2	1.65
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD11	2	1.65
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD12	2	1.65
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD13	2	1.65
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD11	2	1.65
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD12	2	1.65
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD13	2	1.65
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD11	8	1.65
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD12	8	1.65
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD13	8	1.65
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD11	8	1.65
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD12	8	1.65
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD13	8	1.65
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD11	8	1.65
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD12	8	1.65
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD13	8	1.65
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD11	8	1.65
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD12	8	1.65
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD13	8	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD11	8	1.65
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD12	8	1.65
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD13	8	1.65
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD11	8	1.65
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD12	8	1.65
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD13	8	1.65
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD11	1	1.65
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD12	1	1.65
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD13	1	1.65
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD21	1	1.65
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD22	1	1.65
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD23	1	1.65
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD11	5	1.65
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD12	5	1.65
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD13	5	1.65
(5,40)	2:63:B:TRP:CE2	2:62:B:ILE:CG2	2	1.64
(5,40)	2:63:B:TRP:CE2	2:62:B:ILE:CG2	3	1.64
(5,40)	2:63:B:TRP:CE2	2:62:B:ILE:CG2	8	1.64
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD11	8	1.64
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD12	8	1.64
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD13	8	1.64
(1,179)	1:95:A:CYS:SG	1:9:A:GLY:H	7	1.64
(1,97)	1:39:A:CYS:SG	1:75:A:SER:H	5	1.64
(2,41)	1:39:A:CYS:SG	2:64:B:SER:H	10	1.63
(2,36)	1:39:A:CYS:SG	2:58:B:ILE:H	1	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD11	1	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD12	1	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD13	1	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD21	1	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD22	1	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD23	1	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD11	9	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD12	9	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD13	9	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD21	9	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD22	9	1.63
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD23	9	1.63
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD1	3	1.62
(3,36)	2:28:B:THR:CB	2:30:B:LEU:CD2	3	1.62
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD11	3	1.62
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD12	3	1.62
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD13	3	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD11	3	1.62
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD12	3	1.62
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD13	3	1.62
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD11	3	1.62
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD12	3	1.62
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD13	3	1.62
(2,36)	1:39:A:CYS:SG	2:58:B:ILE:H	5	1.62
(2,41)	1:39:A:CYS:SG	2:64:B:SER:H	2	1.61
(2,37)	1:39:A:CYS:SG	2:59:B:ALA:H	2	1.61
(2,28)	1:39:A:CYS:SG	2:43:B:SER:H	7	1.61
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD11	4	1.61
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD12	4	1.61
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD13	4	1.61
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD21	4	1.61
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD22	4	1.61
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD23	4	1.61
(2,36)	1:39:A:CYS:SG	2:58:B:ILE:H	3	1.6
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD11	2	1.6
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD12	2	1.6
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD13	2	1.6
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD21	2	1.6
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD22	2	1.6
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD23	2	1.6
(1,25)	1:5:A:ILE:CG1	1:54:A:ILE:H	9	1.6
(5,40)	2:63:B:TRP:CE2	2:62:B:ILE:CG2	6	1.59
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD11	9	1.59
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD12	9	1.59
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD13	9	1.59
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD11	9	1.59
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD12	9	1.59
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD13	9	1.59
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD11	9	1.59
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD12	9	1.59
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD13	9	1.59
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD11	9	1.59
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD12	9	1.59
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD13	9	1.59
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD11	9	1.59
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD12	9	1.59
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD13	9	1.59
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD11	9	1.59
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD12	9	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD13	9	1.59
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD11	5	1.59
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD12	5	1.59
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD13	5	1.59
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD21	5	1.59
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD22	5	1.59
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD23	5	1.59
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD11	2	1.59
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD12	2	1.59
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD13	2	1.59
(1,97)	1:39:A:CYS:SG	1:75:A:SER:H	2	1.59
(2,75)	1:41:A:CYS:SG	2:8:B:GLY:H	10	1.58
(1,283)	2:5:B:ILE:CG1	2:105:B:SER:H	1	1.58
(5,40)	2:63:B:TRP:CE2	2:62:B:ILE:CG2	4	1.57
(5,11)	2:25:B:GLU:CD	2:22:B:LYS:CE	3	1.57
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD11	3	1.57
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD12	3	1.57
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD13	3	1.57
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD11	3	1.57
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD12	3	1.57
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD13	3	1.57
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD11	3	1.57
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD12	3	1.57
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD13	3	1.57
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD11	8	1.57
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD12	8	1.57
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD13	8	1.57
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD11	10	1.57
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD12	10	1.57
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD13	10	1.57
(5,40)	2:63:B:TRP:CE2	2:62:B:ILE:CG2	1	1.56
(2,75)	1:41:A:CYS:SG	2:8:B:GLY:H	2	1.56
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD11	4	1.56
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD12	4	1.56
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD13	4	1.56
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD21	4	1.56
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD22	4	1.56
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD23	4	1.56
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD11	10	1.56
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD12	10	1.56
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD13	10	1.56
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD11	4	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD12	4	1.55
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD13	4	1.55
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD11	2	1.55
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD12	2	1.55
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD13	2	1.55
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD21	2	1.55
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD22	2	1.55
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD23	2	1.55
(1,200)	1:95:A:CYS:SG	1:59:A:ALA:H	9	1.55
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD11	1	1.54
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD12	1	1.54
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD13	1	1.54
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD21	1	1.54
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD22	1	1.54
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD23	1	1.54
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD11	1	1.54
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD12	1	1.54
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD13	1	1.54
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD21	1	1.54
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD22	1	1.54
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD23	1	1.54
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD11	1	1.54
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD12	1	1.54
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD13	1	1.54
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD21	1	1.54
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD22	1	1.54
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD23	1	1.54
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD11	6	1.54
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD12	6	1.54
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD13	6	1.54
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD11	4	1.54
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD12	4	1.54
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD13	4	1.54
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD21	4	1.54
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD22	4	1.54
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD23	4	1.54
(2,75)	1:41:A:CYS:SG	2:8:B:GLY:H	4	1.54
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD11	9	1.54
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD12	9	1.54
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD13	9	1.54
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD21	9	1.54
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD22	9	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD23	9	1.54
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD11	10	1.54
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD12	10	1.54
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD13	10	1.54
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD21	10	1.54
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD22	10	1.54
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD23	10	1.54
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD11	7	1.54
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD12	7	1.54
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD13	7	1.54
(2,75)	1:41:A:CYS:SG	2:8:B:GLY:H	6	1.53
(2,75)	1:41:A:CYS:SG	2:8:B:GLY:H	9	1.53
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD11	3	1.53
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD12	3	1.53
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD13	3	1.53
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD21	3	1.53
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD22	3	1.53
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD23	3	1.53
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD11	9	1.52
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD12	9	1.52
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD13	9	1.52
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD21	9	1.52
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD22	9	1.52
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD23	9	1.52
(2,308)	2:95:B:CYS:SG	1:107:A:SER:H	8	1.52
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD11	4	1.52
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD12	4	1.52
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD13	4	1.52
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD11	5	1.52
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD12	5	1.52
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD13	5	1.52
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD21	5	1.52
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD22	5	1.52
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD23	5	1.52
(1,296)	2:39:B:CYS:SG	2:24:B:SER:H	4	1.52
(5,11)	2:25:B:GLU:CD	2:22:B:LYS:CE	8	1.51
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD11	7	1.51
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD12	7	1.51
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD13	7	1.51
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD11	7	1.51
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD12	7	1.51
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD13	7	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD11	7	1.51
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD12	7	1.51
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD13	7	1.51
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD11	7	1.51
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD12	7	1.51
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD13	7	1.51
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD11	7	1.51
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD12	7	1.51
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD13	7	1.51
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD11	7	1.51
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD12	7	1.51
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD13	7	1.51
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD11	6	1.51
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD12	6	1.51
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD13	6	1.51
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD11	7	1.5
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD12	7	1.5
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD13	7	1.5
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD11	5	1.5
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD12	5	1.5
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD13	5	1.5
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD21	5	1.5
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD22	5	1.5
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD23	5	1.5
(1,180)	1:95:A:CYS:SG	1:10:A:ALA:H	2	1.5
(6,67)	1:65:A:GLY:O	1:69:A:VAL:H	10	1.49
(5,7)	1:94:A:ILE:CB	2:97:B:GLY:CA	3	1.49
(2,309)	2:95:B:CYS:SG	1:110:A:HIS:H	10	1.49
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD11	10	1.49
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD12	10	1.49
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD13	10	1.49
(1,298)	2:39:B:CYS:SG	2:26:B:GLY:H	7	1.49
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD11	6	1.48
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD12	6	1.48
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD13	6	1.48
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD21	6	1.48
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD22	6	1.48
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD23	6	1.48
(1,300)	2:39:B:CYS:SG	2:28:B:THR:H	9	1.48
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD11	4	1.47
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD12	4	1.47
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD13	4	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD21	4	1.47
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD22	4	1.47
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD23	4	1.47
(1,25)	1:5:A:ILE:CG1	1:54:A:ILE:H	4	1.47
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD11	1	1.46
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD12	1	1.46
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD13	1	1.46
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD11	1	1.46
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD12	1	1.46
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD13	1	1.46
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD11	1	1.46
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD12	1	1.46
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD13	1	1.46
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD11	6	1.46
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD12	6	1.46
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD13	6	1.46
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD21	6	1.46
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD22	6	1.46
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD23	6	1.46
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD11	1	1.46
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD12	1	1.46
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD13	1	1.46
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD21	1	1.46
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD22	1	1.46
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD23	1	1.46
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD11	4	1.46
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD12	4	1.46
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD13	4	1.46
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD21	4	1.46
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD22	4	1.46
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD23	4	1.46
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD11	1	1.46
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD12	1	1.46
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD13	1	1.46
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD21	1	1.46
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD22	1	1.46
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD23	1	1.46
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD11	8	1.46
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD12	8	1.46
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD13	8	1.46
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD11	10	1.45
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD12	10	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD13	10	1.45
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD11	10	1.45
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD12	10	1.45
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD13	10	1.45
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD11	10	1.45
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD12	10	1.45
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD13	10	1.45
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD11	3	1.45
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD12	3	1.45
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD13	3	1.45
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD21	3	1.45
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD22	3	1.45
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD23	3	1.45
(5,117)	1:66:A:VAL:CA	1:68:A:ILE:CD1	10	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD11	2	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD12	2	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD13	2	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD21	2	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD22	2	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD23	2	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD11	5	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD12	5	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD13	5	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD21	5	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD22	5	1.44
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD23	5	1.44
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD11	4	1.43
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD12	4	1.43
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD13	4	1.43
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD11	1	1.43
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD12	1	1.43
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD13	1	1.43
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD21	1	1.43
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD22	1	1.43
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD23	1	1.43
(1,300)	2:39:B:CYS:SG	2:28:B:THR:H	8	1.43
(3,22)	1:54:A:ILE:HD11	1:62:A:ILE:HD11	4	1.42
(3,22)	1:54:A:ILE:HD11	1:62:A:ILE:HD12	4	1.42
(3,22)	1:54:A:ILE:HD11	1:62:A:ILE:HD13	4	1.42
(3,22)	1:54:A:ILE:HD12	1:62:A:ILE:HD11	4	1.42
(3,22)	1:54:A:ILE:HD12	1:62:A:ILE:HD12	4	1.42
(3,22)	1:54:A:ILE:HD12	1:62:A:ILE:HD13	4	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,22)	1:54:A:ILE:HD13	1:62:A:ILE:HD11	4	1.42
(3,22)	1:54:A:ILE:HD13	1:62:A:ILE:HD12	4	1.42
(3,22)	1:54:A:ILE:HD13	1:62:A:ILE:HD13	4	1.42
(1,369)	2:95:B:CYS:SG	2:40:B:TYR:H	1	1.42
(1,97)	1:39:A:CYS:SG	1:75:A:SER:H	1	1.42
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD11	8	1.41
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD12	8	1.41
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD13	8	1.41
(2,35)	1:39:A:CYS:SG	2:57:B:GLY:H	4	1.41
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD11	5	1.4
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD12	5	1.4
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD13	5	1.4
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD11	5	1.4
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD12	5	1.4
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD13	5	1.4
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD11	5	1.4
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD12	5	1.4
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD13	5	1.4
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD11	5	1.4
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD12	5	1.4
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD13	5	1.4
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD11	5	1.4
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD12	5	1.4
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD13	5	1.4
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD11	5	1.4
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD12	5	1.4
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD13	5	1.4
(2,209)	2:39:B:CYS:SG	1:44:A:PHE:H	7	1.4
(2,2)	2:39:B:CYS:SG	2:1:B:MET:HA	6	1.4
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD11	3	1.4
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD12	3	1.4
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD13	3	1.4
(6,68)	1:69:A:VAL:N	1:65:A:GLY:O	10	1.39
(2,37)	1:39:A:CYS:SG	2:59:B:ALA:H	10	1.39
(2,30)	1:39:A:CYS:SG	2:51:B:LEU:H	3	1.39
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD11	7	1.39
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD12	7	1.39
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD13	7	1.39
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD21	7	1.39
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD22	7	1.39
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD23	7	1.39
(6,67)	1:65:A:GLY:O	1:69:A:VAL:H	5	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:39:A:CYS:SG	2:40:B:TYR:H	7	1.38
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD11	9	1.38
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD12	9	1.38
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD13	9	1.38
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD11	6	1.38
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD12	6	1.38
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD13	6	1.38
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD21	6	1.38
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD22	6	1.38
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD23	6	1.38
(1,283)	2:5:B:ILE:CG1	2:105:B:SER:H	8	1.38
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD11	8	1.37
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD12	8	1.37
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD13	8	1.37
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD21	8	1.37
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD22	8	1.37
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD23	8	1.37
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD11	10	1.37
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD12	10	1.37
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD13	10	1.37
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD21	10	1.37
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD22	10	1.37
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD23	10	1.37
(1,301)	2:39:B:CYS:SG	2:29:B:ARG:H	1	1.37
(3,32)	2:71:B:ILE:HD13	3:201:A:P4P:H2D	1	1.36
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD11	6	1.36
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD12	6	1.36
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD13	6	1.36
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD11	6	1.36
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD12	6	1.36
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD13	6	1.36
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD11	6	1.36
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD12	6	1.36
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD13	6	1.36
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD11	6	1.36
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD12	6	1.36
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD13	6	1.36
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD11	6	1.36
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD12	6	1.36
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD13	6	1.36
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD11	6	1.36
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD12	6	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD13	6	1.36
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD11	7	1.36
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD12	7	1.36
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD13	7	1.36
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD21	7	1.36
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD22	7	1.36
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD23	7	1.36
(2,75)	1:41:A:CYS:SG	2:8:B:GLY:H	8	1.36
(2,41)	1:39:A:CYS:SG	2:64:B:SER:H	7	1.36
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD11	7	1.36
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD12	7	1.36
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD13	7	1.36
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD11	6	1.36
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD12	6	1.36
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD13	6	1.36
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD21	6	1.36
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD22	6	1.36
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD23	6	1.36
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD11	5	1.36
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD12	5	1.36
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD13	5	1.36
(1,301)	2:39:B:CYS:SG	2:29:B:ARG:H	4	1.36
(5,117)	1:66:A:VAL:CA	1:68:A:ILE:CD1	7	1.35
(2,205)	2:39:B:CYS:SG	1:37:A:ILE:H	2	1.35
(2,75)	1:41:A:CYS:SG	2:8:B:GLY:H	5	1.35
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD11	9	1.35
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD12	9	1.35
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD13	9	1.35
(1,283)	2:5:B:ILE:CG1	2:105:B:SER:H	5	1.35
(1,25)	1:5:A:ILE:CG1	1:54:A:ILE:H	6	1.35
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG11	1	1.34
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG12	1	1.34
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG13	1	1.34
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG21	1	1.34
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG22	1	1.34
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG23	1	1.34
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG11	1	1.34
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG12	1	1.34
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG13	1	1.34
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG21	1	1.34
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG22	1	1.34
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG23	1	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG11	1	1.34
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG12	1	1.34
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG13	1	1.34
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG21	1	1.34
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG22	1	1.34
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG23	1	1.34
(2,75)	1:41:A:CYS:SG	2:8:B:GLY:H	7	1.34
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD11	8	1.34
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD12	8	1.34
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD13	8	1.34
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD21	8	1.34
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD22	8	1.34
(1,530)	2:39:B:CYS:SG	2:74:B:LEU:HD23	8	1.34
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD11	1	1.34
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD12	1	1.34
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD13	1	1.34
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD11	2	1.33
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD12	2	1.33
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD13	2	1.33
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD11	2	1.33
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD12	2	1.33
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD13	2	1.33
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD11	2	1.33
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD12	2	1.33
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD13	2	1.33
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD11	9	1.33
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD12	9	1.33
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD13	9	1.33
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD21	9	1.33
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD22	9	1.33
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD23	9	1.33
(5,117)	1:66:A:VAL:CA	1:68:A:ILE:CD1	5	1.32
(2,308)	2:95:B:CYS:SG	1:107:A:SER:H	6	1.31
(2,205)	2:39:B:CYS:SG	1:37:A:ILE:H	7	1.31
(2,30)	1:39:A:CYS:SG	2:51:B:LEU:H	6	1.31
(2,29)	1:39:A:CYS:SG	2:49:B:GLN:H	10	1.31
(2,28)	1:39:A:CYS:SG	2:43:B:SER:H	3	1.31
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD11	2	1.31
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD12	2	1.31
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD13	2	1.31
(1,348)	2:95:B:CYS:SG	2:2:B:ASN:H	9	1.31
(1,300)	2:39:B:CYS:SG	2:28:B:THR:H	2	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,29)	1:39:A:CYS:SG	2:49:B:GLN:H	1	1.3
(1,300)	2:39:B:CYS:SG	2:28:B:THR:H	10	1.3
(1,298)	2:39:B:CYS:SG	2:26:B:GLY:H	4	1.3
(1,204)	1:95:A:CYS:SG	1:67:A:GLY:H	8	1.3
(5,117)	1:66:A:VAL:CA	1:68:A:ILE:CD1	9	1.29
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD11	7	1.29
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD12	7	1.29
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD13	7	1.29
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD21	7	1.29
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD22	7	1.29
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD23	7	1.29
(1,283)	2:5:B:ILE:CG1	2:105:B:SER:H	2	1.29
(1,166)	1:41:A:CYS:SG	1:91:A:MET:H	3	1.29
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD11	6	1.28
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD12	6	1.28
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD13	6	1.28
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD21	6	1.28
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD22	6	1.28
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD23	6	1.28
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD11	6	1.28
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD12	6	1.28
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD13	6	1.28
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD21	6	1.28
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD22	6	1.28
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD23	6	1.28
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD11	6	1.28
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD12	6	1.28
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD13	6	1.28
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD21	6	1.28
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD22	6	1.28
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD23	6	1.28
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD11	2	1.28
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD12	2	1.28
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD13	2	1.28
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD21	2	1.28
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD22	2	1.28
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD23	2	1.28
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD11	7	1.28
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD12	7	1.28
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD13	7	1.28
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD21	7	1.28
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD22	7	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD23	7	1.28
(1,296)	2:39:B:CYS:SG	2:24:B:SER:H	5	1.28
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD11	9	1.27
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD12	9	1.27
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD13	9	1.27
(2,205)	2:39:B:CYS:SG	1:37:A:ILE:H	10	1.27
(2,36)	1:39:A:CYS:SG	2:58:B:ILE:H	4	1.27
(2,29)	1:39:A:CYS:SG	2:49:B:GLN:H	2	1.27
(1,480)	1:95:A:CYS:SG	1:5:A:ILE:HD11	10	1.27
(1,480)	1:95:A:CYS:SG	1:5:A:ILE:HD12	10	1.27
(1,480)	1:95:A:CYS:SG	1:5:A:ILE:HD13	10	1.27
(1,97)	1:39:A:CYS:SG	1:75:A:SER:H	4	1.27
(6,68)	1:69:A:VAL:N	1:65:A:GLY:O	5	1.26
(2,29)	1:39:A:CYS:SG	2:49:B:GLN:H	9	1.26
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD11	3	1.26
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD12	3	1.26
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD13	3	1.26
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD21	3	1.26
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD22	3	1.26
(1,443)	1:39:A:CYS:SG	1:51:A:LEU:HD23	3	1.26
(3,32)	2:71:B:ILE:HD13	3:201:A:P4P:H2D	3	1.25
(2,29)	1:39:A:CYS:SG	2:49:B:GLN:H	8	1.25
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD11	3	1.25
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD12	3	1.25
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD13	3	1.25
(1,423)	1:5:A:ILE:CG1	1:58:A:ILE:HD11	7	1.25
(1,423)	1:5:A:ILE:CG1	1:58:A:ILE:HD12	7	1.25
(1,423)	1:5:A:ILE:CG1	1:58:A:ILE:HD13	7	1.25
(3,32)	2:71:B:ILE:HD11	3:201:A:P4P:H2D	8	1.24
(2,36)	1:39:A:CYS:SG	2:58:B:ILE:H	8	1.24
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD11	9	1.24
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD12	9	1.24
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD13	9	1.24
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD11	5	1.24
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD12	5	1.24
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD13	5	1.24
(6,67)	1:65:A:GLY:O	1:69:A:VAL:H	3	1.23
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD11	4	1.23
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD12	4	1.23
(3,2)	2:7:B:LEU:HD11	2:62:B:ILE:HD13	4	1.23
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD11	4	1.23
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD12	4	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	2:7:B:LEU:HD12	2:62:B:ILE:HD13	4	1.23
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD11	4	1.23
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD12	4	1.23
(3,2)	2:7:B:LEU:HD13	2:62:B:ILE:HD13	4	1.23
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD11	4	1.23
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD12	4	1.23
(3,2)	2:7:B:LEU:HD21	2:62:B:ILE:HD13	4	1.23
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD11	4	1.23
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD12	4	1.23
(3,2)	2:7:B:LEU:HD22	2:62:B:ILE:HD13	4	1.23
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD11	4	1.23
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD12	4	1.23
(3,2)	2:7:B:LEU:HD23	2:62:B:ILE:HD13	4	1.23
(2,205)	2:39:B:CYS:SG	1:37:A:ILE:H	5	1.23
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD11	10	1.23
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD12	10	1.23
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD13	10	1.23
(5,117)	1:66:A:VAL:CA	1:68:A:ILE:CD1	2	1.22
(5,7)	1:94:A:ILE:CB	2:97:B:GLY:CA	8	1.22
(3,32)	2:71:B:ILE:HD12	3:201:A:P4P:H2D	6	1.22
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD11	1	1.22
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD12	1	1.22
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD13	1	1.22
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD11	1	1.22
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD12	1	1.22
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD13	1	1.22
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD11	1	1.22
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD12	1	1.22
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD13	1	1.22
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD11	10	1.22
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD12	10	1.22
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD13	10	1.22
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD11	10	1.22
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD12	10	1.22
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD13	10	1.22
(1,296)	2:39:B:CYS:SG	2:24:B:SER:H	10	1.21
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD11	3	1.2
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD12	3	1.2
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD13	3	1.2
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD21	3	1.2
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD22	3	1.2
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD23	3	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:41:A:CYS:SG	1:91:A:MET:H	7	1.2
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD11	4	1.19
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD12	4	1.19
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD13	4	1.19
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD11	4	1.19
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD12	4	1.19
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD13	4	1.19
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD11	4	1.19
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD12	4	1.19
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD13	4	1.19
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD11	9	1.19
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD12	9	1.19
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD13	9	1.19
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD21	9	1.19
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD22	9	1.19
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD23	9	1.19
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD11	5	1.19
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD12	5	1.19
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD13	5	1.19
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD11	1	1.19
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD12	1	1.19
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD13	1	1.19
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD11	9	1.19
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD12	9	1.19
(1,477)	1:41:A:CYS:SG	1:94:A:ILE:HD13	9	1.19
(1,218)	1:95:A:CYS:SG	1:88:A:ILE:H	5	1.19
(6,68)	1:69:A:VAL:N	1:65:A:GLY:O	3	1.18
(5,117)	1:66:A:VAL:CA	1:68:A:ILE:CD1	4	1.18
(5,5)	2:90:B:GLY:CA	1:97:A:GLY:CA	1	1.18
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD11	2	1.18
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD12	2	1.18
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD13	2	1.18
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD11	2	1.18
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD12	2	1.18
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD13	2	1.18
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD11	2	1.18
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD12	2	1.18
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD13	2	1.18
(1,218)	1:95:A:CYS:SG	1:88:A:ILE:H	2	1.18
(1,218)	1:95:A:CYS:SG	1:88:A:ILE:H	4	1.17
(1,25)	1:5:A:ILE:CG1	1:54:A:ILE:H	5	1.17
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD11	10	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD12	10	1.16
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD13	10	1.16
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD11	10	1.16
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD12	10	1.16
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD13	10	1.16
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD11	10	1.16
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD12	10	1.16
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD13	10	1.16
(2,209)	2:39:B:CYS:SG	1:44:A:PHE:H	3	1.16
(2,30)	1:39:A:CYS:SG	2:51:B:LEU:H	2	1.16
(5,9)	2:10:B:ALA:CA	2:11:B:ILE:CD1	6	1.15
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD11	2	1.15
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD12	2	1.15
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD13	2	1.15
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD11	2	1.15
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD12	2	1.15
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD13	2	1.15
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD11	2	1.15
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD12	2	1.15
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD13	2	1.15
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD11	8	1.15
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD12	8	1.15
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD13	8	1.15
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD21	8	1.15
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD22	8	1.15
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD23	8	1.15
(2,41)	1:39:A:CYS:SG	2:64:B:SER:H	3	1.15
(1,180)	1:95:A:CYS:SG	1:10:A:ALA:H	4	1.15
(1,369)	2:95:B:CYS:SG	2:40:B:TYR:H	8	1.14
(1,303)	2:39:B:CYS:SG	2:31:B:TRP:H	1	1.14
(1,298)	2:39:B:CYS:SG	2:26:B:GLY:H	1	1.14
(1,283)	2:5:B:ILE:CG1	2:105:B:SER:H	6	1.14
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD11	3	1.13
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD12	3	1.13
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD13	3	1.13
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD21	3	1.13
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD22	3	1.13
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD23	3	1.13
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD11	3	1.13
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD12	3	1.13
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD13	3	1.13
(1,166)	1:41:A:CYS:SG	1:91:A:MET:H	2	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD11	7	1.12
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD12	7	1.12
(1,537)	2:39:B:CYS:SG	2:101:B:ILE:HD13	7	1.12
(5,134)	1:90:A:GLY:CA	1:86:A:PRO:CD	9	1.11
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD11	8	1.11
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD12	8	1.11
(2,394)	1:39:A:CYS:SG	2:58:B:ILE:HD13	8	1.11
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD11	9	1.11
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD12	9	1.11
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD13	9	1.11
(2,209)	2:39:B:CYS:SG	1:44:A:PHE:H	8	1.1
(5,9)	2:10:B:ALA:CA	2:11:B:ILE:CD1	7	1.09
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD11	1	1.09
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD12	1	1.09
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD13	1	1.09
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD21	1	1.09
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD22	1	1.09
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD23	1	1.09
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD11	8	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD12	8	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD13	8	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD21	8	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD22	8	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD23	8	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD11	9	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD12	9	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD13	9	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD21	9	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD22	9	1.08
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD23	9	1.08
(1,369)	2:95:B:CYS:SG	2:40:B:TYR:H	7	1.08
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD11	7	1.07
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD12	7	1.07
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD13	7	1.07
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD11	8	1.06
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD12	8	1.06
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD13	8	1.06
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD21	8	1.06
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD22	8	1.06
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD23	8	1.06
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD11	8	1.06
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD12	8	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD13	8	1.06
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD21	8	1.06
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD22	8	1.06
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD23	8	1.06
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD11	8	1.06
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD12	8	1.06
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD13	8	1.06
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD21	8	1.06
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD22	8	1.06
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD23	8	1.06
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD11	4	1.06
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD12	4	1.06
(3,8)	2:62:B:ILE:HD11	2:11:B:ILE:HD13	4	1.06
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD11	4	1.06
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD12	4	1.06
(3,8)	2:62:B:ILE:HD12	2:11:B:ILE:HD13	4	1.06
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD11	4	1.06
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD12	4	1.06
(3,8)	2:62:B:ILE:HD13	2:11:B:ILE:HD13	4	1.06
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD11	9	1.06
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD12	9	1.06
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD13	9	1.06
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD11	9	1.06
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD12	9	1.06
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD13	9	1.06
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD11	9	1.06
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD12	9	1.06
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD13	9	1.06
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD11	9	1.06
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD12	9	1.06
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD13	9	1.06
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD11	9	1.06
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD12	9	1.06
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD13	9	1.06
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD11	9	1.06
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD12	9	1.06
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD13	9	1.06
(2,41)	1:39:A:CYS:SG	2:64:B:SER:H	4	1.06
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD11	3	1.06
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD12	3	1.06
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD13	3	1.06
(1,480)	1:95:A:CYS:SG	1:5:A:ILE:HD11	6	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:95:A:CYS:SG	1:5:A:ILE:HD12	6	1.06
(1,480)	1:95:A:CYS:SG	1:5:A:ILE:HD13	6	1.06
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD11	10	1.06
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD12	10	1.06
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD13	10	1.06
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD21	10	1.06
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD22	10	1.06
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD23	10	1.06
(1,166)	1:41:A:CYS:SG	1:91:A:MET:H	8	1.06
(3,33)	1:47:A:LEU:HD11	3:201:A:P4P:H2C	5	1.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD11	3	1.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD12	3	1.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD13	3	1.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD21	3	1.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD22	3	1.03
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD23	3	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD11	3	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD12	3	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD13	3	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD21	3	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD22	3	1.03
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD23	3	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD11	3	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD12	3	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD13	3	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD21	3	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD22	3	1.03
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD23	3	1.03
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD11	8	1.03
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD12	8	1.03
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD13	8	1.03
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD21	8	1.03
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD22	8	1.03
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD23	8	1.03
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD11	6	1.03
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD12	6	1.03
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD13	6	1.03
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD21	6	1.03
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD22	6	1.03
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD23	6	1.03
(2,308)	2:95:B:CYS:SG	1:107:A:SER:H	10	1.03
(2,30)	1:39:A:CYS:SG	2:51:B:LEU:H	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,28)	1:39:A:CYS:SG	2:43:B:SER:H	5	1.03
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD11	9	1.03
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD12	9	1.03
(1,489)	1:95:A:CYS:SG	1:58:A:ILE:HD13	9	1.03
(1,25)	1:5:A:ILE:CG1	1:54:A:ILE:H	1	1.03
(3,32)	2:71:B:ILE:HD12	3:201:A:P4P:H2B	5	1.02
(2,158)	2:30:B:LEU:CG	1:45:A:TRP:H	10	1.02
(2,29)	1:39:A:CYS:SG	2:49:B:GLN:H	4	1.02
(2,205)	2:39:B:CYS:SG	1:37:A:ILE:H	4	1.01
(2,37)	1:39:A:CYS:SG	2:59:B:ALA:H	9	1.01
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD11	10	1.01
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD12	10	1.01
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD13	10	1.01
(1,296)	2:39:B:CYS:SG	2:24:B:SER:H	8	1.01
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD11	8	1.0
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD12	8	1.0
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD13	8	1.0
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD21	8	1.0
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD22	8	1.0
(1,486)	1:95:A:CYS:SG	1:46:A:LEU:HD23	8	1.0
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD11	5	1.0
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD12	5	1.0
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD13	5	1.0
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD21	5	1.0
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD22	5	1.0
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD23	5	1.0
(1,296)	2:39:B:CYS:SG	2:24:B:SER:H	9	1.0
(1,180)	1:95:A:CYS:SG	1:10:A:ALA:H	5	1.0
(2,37)	1:39:A:CYS:SG	2:59:B:ALA:H	6	0.99
(2,30)	1:39:A:CYS:SG	2:51:B:LEU:H	5	0.99
(1,320)	2:39:B:CYS:SG	2:64:B:SER:H	4	0.99
(2,28)	1:39:A:CYS:SG	2:43:B:SER:H	8	0.98
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD11	8	0.98
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD12	8	0.98
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD13	8	0.98
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD21	8	0.98
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD22	8	0.98
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD23	8	0.98
(1,348)	2:95:B:CYS:SG	2:2:B:ASN:H	3	0.98
(1,177)	1:95:A:CYS:SG	1:7:A:LEU:H	6	0.98
(1,25)	1:5:A:ILE:CG1	1:54:A:ILE:H	2	0.98
(5,5)	2:90:B:GLY:CA	1:97:A:GLY:CA	6	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD11	4	0.97
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD12	4	0.97
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD13	4	0.97
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD21	4	0.97
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD22	4	0.97
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD23	4	0.97
(6,65)	1:64:A:SER:O	1:68:A:ILE:H	8	0.96
(5,134)	1:90:A:GLY:CA	1:86:A:PRO:CD	7	0.96
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD11	7	0.96
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD12	7	0.96
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD13	7	0.96
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD11	7	0.96
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD12	7	0.96
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD13	7	0.96
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD11	7	0.96
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD12	7	0.96
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD13	7	0.96
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD11	2	0.96
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD12	2	0.96
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD13	2	0.96
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD11	10	0.96
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD12	10	0.96
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD13	10	0.96
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD11	7	0.95
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD12	7	0.95
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD13	7	0.95
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD21	7	0.95
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD22	7	0.95
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD23	7	0.95
(2,308)	2:95:B:CYS:SG	1:107:A:SER:H	1	0.95
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD11	2	0.95
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD12	2	0.95
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD13	2	0.95
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD11	7	0.95
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD12	7	0.95
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD13	7	0.95
(1,301)	2:39:B:CYS:SG	2:29:B:ARG:H	6	0.95
(6,67)	1:65:A:GLY:O	1:69:A:VAL:H	1	0.94
(6,66)	1:68:A:ILE:N	1:64:A:SER:O	8	0.94
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD11	4	0.94
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD12	4	0.94
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD13	4	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD21	4	0.94
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD22	4	0.94
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD23	4	0.94
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD11	4	0.94
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD12	4	0.94
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD13	4	0.94
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD21	4	0.94
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD22	4	0.94
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD23	4	0.94
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD11	4	0.94
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD12	4	0.94
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD13	4	0.94
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD21	4	0.94
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD22	4	0.94
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD23	4	0.94
(1,179)	1:95:A:CYS:SG	1:9:A:GLY:H	2	0.94
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD11	8	0.93
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD12	8	0.93
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD13	8	0.93
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD11	8	0.93
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD12	8	0.93
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD13	8	0.93
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD11	8	0.93
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD12	8	0.93
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD13	8	0.93
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD11	10	0.93
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD12	10	0.93
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD13	10	0.93
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD11	4	0.93
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD12	4	0.93
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD13	4	0.93
(6,65)	1:64:A:SER:O	1:68:A:ILE:H	5	0.92
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD11	9	0.92
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD12	9	0.92
(3,7)	2:58:B:ILE:HD11	2:54:B:ILE:HD13	9	0.92
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD11	9	0.92
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD12	9	0.92
(3,7)	2:58:B:ILE:HD12	2:54:B:ILE:HD13	9	0.92
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD11	9	0.92
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD12	9	0.92
(3,7)	2:58:B:ILE:HD13	2:54:B:ILE:HD13	9	0.92
(6,68)	1:69:A:VAL:N	1:65:A:GLY:O	1	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,65)	1:64:A:SER:O	1:68:A:ILE:H	10	0.91
(5,134)	1:90:A:GLY:CA	1:86:A:PRO:CD	3	0.91
(2,41)	1:39:A:CYS:SG	2:64:B:SER:H	6	0.91
(2,27)	1:39:A:CYS:SG	2:40:B:TYR:H	10	0.91
(1,25)	1:5:A:ILE:CG1	1:54:A:ILE:H	3	0.91
(5,134)	1:90:A:GLY:CA	1:86:A:PRO:CD	5	0.9
(2,309)	2:95:B:CYS:SG	1:110:A:HIS:H	6	0.9
(2,209)	2:39:B:CYS:SG	1:44:A:PHE:H	4	0.9
(3,33)	1:47:A:LEU:HD11	3:201:A:P4P:H2B	6	0.89
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD11	1	0.89
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD12	1	0.89
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD13	1	0.89
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD21	1	0.89
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD22	1	0.89
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD23	1	0.89
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD11	1	0.89
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD12	1	0.89
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD13	1	0.89
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD21	1	0.89
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD22	1	0.89
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD23	1	0.89
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD11	1	0.89
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD12	1	0.89
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD13	1	0.89
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD21	1	0.89
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD22	1	0.89
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD23	1	0.89
(2,309)	2:95:B:CYS:SG	1:110:A:HIS:H	7	0.89
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD11	7	0.89
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD12	7	0.89
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD13	7	0.89
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD21	7	0.89
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD22	7	0.89
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD23	7	0.89
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD11	3	0.88
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD12	3	0.88
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD13	3	0.88
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD11	10	0.88
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD12	10	0.88
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD13	10	0.88
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD21	10	0.88
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD22	10	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD23	10	0.88
(2,75)	1:41:A:CYS:SG	2:8:B:GLY:H	1	0.88
(2,30)	1:39:A:CYS:SG	2:51:B:LEU:H	9	0.88
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD11	3	0.88
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD12	3	0.88
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD13	3	0.88
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD21	3	0.88
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD22	3	0.88
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD23	3	0.88
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD11	7	0.88
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD12	7	0.88
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD13	7	0.88
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD11	2	0.88
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD12	2	0.88
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD13	2	0.88
(1,296)	2:39:B:CYS:SG	2:24:B:SER:H	2	0.88
(6,66)	1:68:A:ILE:N	1:64:A:SER:O	5	0.87
(5,134)	1:90:A:GLY:CA	1:86:A:PRO:CD	10	0.87
(5,10)	2:11:B:ILE:CD1	2:63:B:TRP:CA	1	0.87
(5,7)	1:94:A:ILE:CB	2:97:B:GLY:CA	6	0.87
(2,308)	2:95:B:CYS:SG	1:107:A:SER:H	3	0.87
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD11	2	0.87
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD12	2	0.87
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD13	2	0.87
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD11	6	0.87
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD12	6	0.87
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD13	6	0.87
(1,180)	1:95:A:CYS:SG	1:10:A:ALA:H	1	0.87
(6,66)	1:68:A:ILE:N	1:64:A:SER:O	10	0.86
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD11	10	0.86
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD12	10	0.86
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD13	10	0.86
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD21	10	0.86
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD22	10	0.86
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD23	10	0.86
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD11	2	0.86
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD12	2	0.86
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD13	2	0.86
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD21	2	0.86
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD22	2	0.86
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD23	2	0.86
(5,9)	2:10:B:ALA:CA	2:11:B:ILE:CD1	5	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1)	1:93:A:LEU:CB	2:97:B:GLY:CA	4	0.85
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD11	4	0.85
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD12	4	0.85
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD13	4	0.85
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD21	4	0.85
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD22	4	0.85
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD23	4	0.85
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD11	9	0.85
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD12	9	0.85
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD13	9	0.85
(6,101)	1:95:A:CYS:O	1:99:A:LEU:H	1	0.84
(6,65)	1:64:A:SER:O	1:68:A:ILE:H	2	0.84
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD11	9	0.84
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD12	9	0.84
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD13	9	0.84
(2,209)	2:39:B:CYS:SG	1:44:A:PHE:H	1	0.84
(2,209)	2:39:B:CYS:SG	1:44:A:PHE:H	5	0.84
(2,37)	1:39:A:CYS:SG	2:59:B:ALA:H	3	0.84
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD11	4	0.84
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD12	4	0.84
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD13	4	0.84
(5,9)	2:10:B:ALA:CA	2:11:B:ILE:CD1	1	0.83
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD11	10	0.83
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD12	10	0.83
(2,475)	2:95:B:CYS:SG	1:100:A:ILE:HD13	10	0.83
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD11	4	0.83
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD12	4	0.83
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD13	4	0.83
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD21	4	0.83
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD22	4	0.83
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD23	4	0.83
(1,301)	2:39:B:CYS:SG	2:29:B:ARG:H	7	0.83
(1,296)	2:39:B:CYS:SG	2:24:B:SER:H	6	0.83
(1,179)	1:95:A:CYS:SG	1:9:A:GLY:H	1	0.83
(5,134)	1:90:A:GLY:CA	1:86:A:PRO:CD	2	0.82
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD11	7	0.82
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD12	7	0.82
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD13	7	0.82
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD11	5	0.82
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD12	5	0.82
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD13	5	0.82
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD21	5	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD22	5	0.82
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD23	5	0.82
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD11	4	0.82
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD12	4	0.82
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD13	4	0.82
(1,301)	2:39:B:CYS:SG	2:29:B:ARG:H	5	0.82
(6,102)	1:99:A:LEU:N	1:95:A:CYS:O	1	0.81
(5,5)	2:90:B:GLY:CA	1:97:A:GLY:CA	8	0.81
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD11	4	0.81
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD12	4	0.81
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD13	4	0.81
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD21	4	0.81
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD22	4	0.81
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD23	4	0.81
(2,27)	1:39:A:CYS:SG	2:40:B:TYR:H	5	0.81
(1,220)	1:95:A:CYS:SG	1:90:A:GLY:H	8	0.81
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD11	2	0.8
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD12	2	0.8
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD13	2	0.8
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD21	2	0.8
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD22	2	0.8
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD23	2	0.8
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD11	2	0.8
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD12	2	0.8
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD13	2	0.8
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD21	2	0.8
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD22	2	0.8
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD23	2	0.8
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD11	2	0.8
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD12	2	0.8
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD13	2	0.8
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD21	2	0.8
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD22	2	0.8
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD23	2	0.8
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD11	10	0.8
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD12	10	0.8
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD13	10	0.8
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD21	10	0.8
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD22	10	0.8
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD23	10	0.8
(2,205)	2:39:B:CYS:SG	1:37:A:ILE:H	6	0.8
(2,28)	1:39:A:CYS:SG	2:43:B:SER:H	10	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD11	1	0.8
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD12	1	0.8
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD13	1	0.8
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD11	2	0.8
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD12	2	0.8
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD13	2	0.8
(1,166)	1:41:A:CYS:SG	1:91:A:MET:H	1	0.8
(6,67)	1:65:A:GLY:O	1:69:A:VAL:H	2	0.79
(6,65)	1:64:A:SER:O	1:68:A:ILE:H	9	0.79
(3,34)	1:47:A:LEU:HD12	3:201:A:P4P:H2A	4	0.79
(2,205)	2:39:B:CYS:SG	1:37:A:ILE:H	8	0.79
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD11	3	0.79
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD12	3	0.79
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD13	3	0.79
(6,66)	1:68:A:ILE:N	1:64:A:SER:O	2	0.78
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD11	7	0.78
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD12	7	0.78
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD13	7	0.78
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD21	7	0.78
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD22	7	0.78
(2,440)	2:41:B:CYS:SG	1:7:A:LEU:HD23	7	0.78
(2,209)	2:39:B:CYS:SG	1:44:A:PHE:H	10	0.78
(2,27)	1:39:A:CYS:SG	2:40:B:TYR:H	2	0.78
(1,303)	2:39:B:CYS:SG	2:31:B:TRP:H	4	0.78
(1,283)	2:5:B:ILE:CG1	2:105:B:SER:H	4	0.78
(1,283)	2:5:B:ILE:CG1	2:105:B:SER:H	10	0.78
(5,134)	1:90:A:GLY:CA	1:86:A:PRO:CD	1	0.77
(5,5)	2:90:B:GLY:CA	1:97:A:GLY:CA	3	0.77
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD11	5	0.77
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD12	5	0.77
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD13	5	0.77
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD11	9	0.77
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD12	9	0.77
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD13	9	0.77
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD21	9	0.77
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD22	9	0.77
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD23	9	0.77
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD11	8	0.77
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD12	8	0.77
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD13	8	0.77
(5,134)	1:90:A:GLY:CA	1:86:A:PRO:CD	4	0.76
(5,134)	1:90:A:GLY:CA	1:86:A:PRO:CD	8	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,5)	2:90:B:GLY:CA	1:97:A:GLY:CA	4	0.76
(2,30)	1:39:A:CYS:SG	2:51:B:LEU:H	8	0.76
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD11	7	0.76
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD12	7	0.76
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD13	7	0.76
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD11	2	0.76
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD12	2	0.76
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD13	2	0.76
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD21	2	0.76
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD22	2	0.76
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD23	2	0.76
(1,201)	1:95:A:CYS:SG	1:60:A:TYR:H	5	0.76
(6,67)	1:65:A:GLY:O	1:69:A:VAL:H	8	0.75
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD11	7	0.75
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD12	7	0.75
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD13	7	0.75
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD21	7	0.75
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD22	7	0.75
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD23	7	0.75
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD11	7	0.75
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD12	7	0.75
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD13	7	0.75
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD21	7	0.75
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD22	7	0.75
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD23	7	0.75
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD11	7	0.75
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD12	7	0.75
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD13	7	0.75
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD21	7	0.75
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD22	7	0.75
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD23	7	0.75
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD11	5	0.75
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD12	5	0.75
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD13	5	0.75
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD21	5	0.75
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD22	5	0.75
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD23	5	0.75
(1,201)	1:95:A:CYS:SG	1:60:A:TYR:H	6	0.75
(6,68)	1:69:A:VAL:N	1:65:A:GLY:O	2	0.74
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD11	8	0.74
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD12	8	0.74
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD13	8	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD21	8	0.74
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD22	8	0.74
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD23	8	0.74
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD11	8	0.74
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD12	8	0.74
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD13	8	0.74
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD21	8	0.74
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD22	8	0.74
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD23	8	0.74
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD11	8	0.74
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD12	8	0.74
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD13	8	0.74
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD21	8	0.74
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD22	8	0.74
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD23	8	0.74
(1,348)	2:95:B:CYS:SG	2:2:B:ASN:H	2	0.74
(6,66)	1:68:A:ILE:N	1:64:A:SER:O	9	0.73
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD11	8	0.73
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD12	8	0.73
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD13	8	0.73
(3,34)	1:47:A:LEU:HD12	3:201:A:P4P:H2C	9	0.72
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD11	3	0.72
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD12	3	0.72
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD13	3	0.72
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD11	3	0.72
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD12	3	0.72
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD13	3	0.72
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD11	3	0.72
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD12	3	0.72
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD13	3	0.72
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD11	3	0.72
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD12	3	0.72
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD13	3	0.72
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD11	3	0.72
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD12	3	0.72
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD13	3	0.72
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD11	3	0.72
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD12	3	0.72
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD13	3	0.72
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD11	8	0.72
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD12	8	0.72
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD13	8	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:95:A:CYS:SG	1:57:A:GLY:H	6	0.72
(1,179)	1:95:A:CYS:SG	1:9:A:GLY:H	5	0.72
(6,68)	1:69:A:VAL:N	1:65:A:GLY:O	8	0.71
(2,27)	1:39:A:CYS:SG	2:40:B:TYR:H	8	0.71
(2,28)	1:39:A:CYS:SG	2:43:B:SER:H	2	0.7
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD11	1	0.7
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD12	1	0.7
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD13	1	0.7
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD21	1	0.7
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD22	1	0.7
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD23	1	0.7
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD11	3	0.69
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD12	3	0.69
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD13	3	0.69
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD21	3	0.69
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD22	3	0.69
(2,426)	2:39:B:CYS:SG	1:30:A:LEU:HD23	3	0.69
(2,308)	2:95:B:CYS:SG	1:107:A:SER:H	9	0.69
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD11	9	0.69
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD12	9	0.69
(1,529)	2:39:B:CYS:SG	2:71:B:ILE:HD13	9	0.69
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD11	2	0.69
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD12	2	0.69
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD13	2	0.69
(5,35)	2:28:B:THR:CB	2:30:B:LEU:CA	5	0.68
(3,32)	2:71:B:ILE:HD11	3:201:A:P4P:H2D	7	0.68
(2,28)	1:39:A:CYS:SG	2:43:B:SER:H	6	0.68
(2,27)	1:39:A:CYS:SG	2:40:B:TYR:H	3	0.68
(1,492)	1:95:A:CYS:SG	1:71:A:ILE:HD11	4	0.68
(1,492)	1:95:A:CYS:SG	1:71:A:ILE:HD12	4	0.68
(1,492)	1:95:A:CYS:SG	1:71:A:ILE:HD13	4	0.68
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD11	6	0.68
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD12	6	0.68
(1,456)	1:39:A:CYS:SG	1:94:A:ILE:HD13	6	0.68
(1,301)	2:39:B:CYS:SG	2:29:B:ARG:H	3	0.68
(5,134)	1:90:A:GLY:CA	1:86:A:PRO:CD	6	0.67
(5,7)	1:94:A:ILE:CB	2:97:B:GLY:CA	7	0.67
(3,38)	2:63:B:TRP:CD1	2:47:B:LEU:CD1	8	0.67
(3,38)	2:63:B:TRP:CD1	2:47:B:LEU:CD2	8	0.67
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD11	2	0.67
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD12	2	0.67
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD13	2	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD21	2	0.67
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD22	2	0.67
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD23	2	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD11	2	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD12	2	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD13	2	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD21	2	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD22	2	0.67
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD23	2	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD11	2	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD12	2	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD13	2	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD21	2	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD22	2	0.67
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD23	2	0.67
(2,205)	2:39:B:CYS:SG	1:37:A:ILE:H	9	0.67
(1,298)	2:39:B:CYS:SG	2:26:B:GLY:H	5	0.67
(1,220)	1:95:A:CYS:SG	1:90:A:GLY:H	1	0.67
(1,182)	1:95:A:CYS:SG	1:14:A:GLU:H	9	0.67
(1,179)	1:95:A:CYS:SG	1:9:A:GLY:H	4	0.67
(5,5)	2:90:B:GLY:CA	1:97:A:GLY:CA	9	0.66
(3,33)	1:47:A:LEU:HD11	3:201:A:P4P:H2A	10	0.66
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD11	2	0.66
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD12	2	0.66
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD13	2	0.66
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD11	2	0.66
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD12	2	0.66
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD13	2	0.66
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD11	2	0.66
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD12	2	0.66
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD13	2	0.66
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD11	2	0.66
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD12	2	0.66
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD13	2	0.66
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD11	2	0.66
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD12	2	0.66
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD13	2	0.66
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD11	2	0.66
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD12	2	0.66
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD13	2	0.66
(2,41)	1:39:A:CYS:SG	2:64:B:SER:H	5	0.66
(2,37)	1:39:A:CYS:SG	2:59:B:ALA:H	4	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD11	8	0.66
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD12	8	0.66
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD13	8	0.66
(1,492)	1:95:A:CYS:SG	1:71:A:ILE:HD11	2	0.66
(1,492)	1:95:A:CYS:SG	1:71:A:ILE:HD12	2	0.66
(1,492)	1:95:A:CYS:SG	1:71:A:ILE:HD13	2	0.66
(6,155)	2:43:B:SER:O	2:47:B:LEU:H	2	0.65
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD11	3	0.65
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD12	3	0.65
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD13	3	0.65
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD21	3	0.65
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD22	3	0.65
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD23	3	0.65
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD11	3	0.65
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD12	3	0.65
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD13	3	0.65
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD21	3	0.65
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD22	3	0.65
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD23	3	0.65
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD11	3	0.65
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD12	3	0.65
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD13	3	0.65
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD21	3	0.65
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD22	3	0.65
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD23	3	0.65
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD11	5	0.65
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD12	5	0.65
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD13	5	0.65
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD21	5	0.65
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD22	5	0.65
(1,472)	1:41:A:CYS:SG	1:74:A:LEU:HD23	5	0.65
(1,369)	2:95:B:CYS:SG	2:40:B:TYR:H	3	0.65
(6,65)	1:64:A:SER:O	1:68:A:ILE:H	6	0.64
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD11	7	0.64
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD12	7	0.64
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD13	7	0.64
(2,41)	1:39:A:CYS:SG	2:64:B:SER:H	9	0.64
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD11	8	0.64
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD12	8	0.64
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD13	8	0.64
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD21	8	0.64
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD22	8	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD23	8	0.64
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD11	4	0.64
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD12	4	0.64
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD13	4	0.64
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD21	4	0.64
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD22	4	0.64
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD23	4	0.64
(1,284)	2:5:B:ILE:CG1	2:106:B:ARG:H	5	0.64
(1,201)	1:95:A:CYS:SG	1:60:A:TYR:H	7	0.64
(6,155)	2:43:B:SER:O	2:47:B:LEU:H	10	0.63
(6,66)	1:68:A:ILE:N	1:64:A:SER:O	6	0.63
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD11	5	0.63
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD12	5	0.63
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD13	5	0.63
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD21	5	0.63
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD22	5	0.63
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD23	5	0.63
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD11	10	0.63
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD12	10	0.63
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD13	10	0.63
(2,209)	2:39:B:CYS:SG	1:44:A:PHE:H	9	0.63
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD11	7	0.62
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD12	7	0.62
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD13	7	0.62
(1,176)	1:95:A:CYS:SG	1:6:A:TYR:H	10	0.62
(3,40)	2:63:B:TRP:CE2	2:66:B:VAL:CG1	10	0.61
(3,40)	2:63:B:TRP:CE2	2:66:B:VAL:CG2	10	0.61
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD11	4	0.61
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD12	4	0.61
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD13	4	0.61
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD11	4	0.61
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD12	4	0.61
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD13	4	0.61
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD11	4	0.61
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD12	4	0.61
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD13	4	0.61
(2,37)	1:39:A:CYS:SG	2:59:B:ALA:H	1	0.61
(2,30)	1:39:A:CYS:SG	2:51:B:LEU:H	10	0.61
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD11	8	0.61
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD12	8	0.61
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD13	8	0.61
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD21	8	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD22	8	0.61
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD23	8	0.61
(5,9)	2:10:B:ALA:CA	2:11:B:ILE:CD1	8	0.6
(5,6)	1:90:A:GLY:CA	2:97:B:GLY:CA	4	0.6
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD11	6	0.6
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD12	6	0.6
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD13	6	0.6
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD21	6	0.6
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD22	6	0.6
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD23	6	0.6
(2,309)	2:95:B:CYS:SG	1:110:A:HIS:H	8	0.6
(2,37)	1:39:A:CYS:SG	2:59:B:ALA:H	5	0.6
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD11	6	0.6
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD12	6	0.6
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD13	6	0.6
(6,67)	1:65:A:GLY:O	1:69:A:VAL:H	4	0.59
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD11	1	0.59
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD12	1	0.59
(2,396)	1:39:A:CYS:SG	2:68:B:ILE:HD13	1	0.59
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD11	3	0.59
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD12	3	0.59
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD13	3	0.59
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD21	3	0.59
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD22	3	0.59
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD23	3	0.59
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD11	5	0.59
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD12	5	0.59
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD13	5	0.59
(1,201)	1:95:A:CYS:SG	1:60:A:TYR:H	2	0.59
(1,182)	1:95:A:CYS:SG	1:14:A:GLU:H	10	0.59
(5,81)	1:43:A:SER:CA	1:45:A:TRP:CD2	3	0.58
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD11	2	0.58
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD12	2	0.58
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD13	2	0.58
(1,423)	1:5:A:ILE:CG1	1:58:A:ILE:HD11	9	0.58
(1,423)	1:5:A:ILE:CG1	1:58:A:ILE:HD12	9	0.58
(1,423)	1:5:A:ILE:CG1	1:58:A:ILE:HD13	9	0.58
(1,301)	2:39:B:CYS:SG	2:29:B:ARG:H	8	0.58
(1,199)	1:95:A:CYS:SG	1:57:A:GLY:H	5	0.58
(6,27)	1:33:A:SER:O	1:37:A:ILE:H	6	0.57
(5,130)	1:87:A:ALA:CA	1:85:A:LEU:CG	10	0.57
(5,95)	1:63:A:TRP:CA	1:14:A:GLU:CD	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,5)	2:90:B:GLY:CA	1:97:A:GLY:CA	2	0.57
(4,1)	1:14:A:GLU:OE1	2:60:B:TYR:OH	5	0.57
(3,23)	1:58:A:ILE:HD11	1:62:A:ILE:HD11	4	0.57
(3,23)	1:58:A:ILE:HD11	1:62:A:ILE:HD12	4	0.57
(3,23)	1:58:A:ILE:HD11	1:62:A:ILE:HD13	4	0.57
(3,23)	1:58:A:ILE:HD12	1:62:A:ILE:HD11	4	0.57
(3,23)	1:58:A:ILE:HD12	1:62:A:ILE:HD12	4	0.57
(3,23)	1:58:A:ILE:HD12	1:62:A:ILE:HD13	4	0.57
(3,23)	1:58:A:ILE:HD13	1:62:A:ILE:HD11	4	0.57
(3,23)	1:58:A:ILE:HD13	1:62:A:ILE:HD12	4	0.57
(3,23)	1:58:A:ILE:HD13	1:62:A:ILE:HD13	4	0.57
(2,205)	2:39:B:CYS:SG	1:37:A:ILE:H	1	0.57
(2,28)	1:39:A:CYS:SG	2:43:B:SER:H	9	0.57
(3,39)	2:63:B:TRP:CE2	2:47:B:LEU:CD1	8	0.56
(3,39)	2:63:B:TRP:CE2	2:47:B:LEU:CD2	8	0.56
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD11	6	0.56
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD12	6	0.56
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD13	6	0.56
(2,205)	2:39:B:CYS:SG	1:37:A:ILE:H	3	0.56
(2,41)	1:39:A:CYS:SG	2:64:B:SER:H	1	0.56
(1,348)	2:95:B:CYS:SG	2:2:B:ASN:H	8	0.56
(1,303)	2:39:B:CYS:SG	2:31:B:TRP:H	3	0.56
(1,303)	2:39:B:CYS:SG	2:31:B:TRP:H	8	0.56
(1,199)	1:95:A:CYS:SG	1:57:A:GLY:H	7	0.56
(6,153)	2:42:B:ALA:O	2:46:B:LEU:H	2	0.55
(6,65)	1:64:A:SER:O	1:68:A:ILE:H	1	0.55
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD11	10	0.55
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD12	10	0.55
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD13	10	0.55
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD11	10	0.55
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD12	10	0.55
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD13	10	0.55
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD11	10	0.55
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD12	10	0.55
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD13	10	0.55
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD11	10	0.55
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD12	10	0.55
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD13	10	0.55
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD11	10	0.55
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD12	10	0.55
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD13	10	0.55
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD11	10	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD12	10	0.55
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD13	10	0.55
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD11	10	0.55
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD12	10	0.55
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD13	10	0.55
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD11	10	0.55
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD12	10	0.55
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD13	10	0.55
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD11	10	0.55
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD12	10	0.55
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD13	10	0.55
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD11	10	0.55
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD12	10	0.55
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD13	10	0.55
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD11	10	0.55
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD12	10	0.55
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD13	10	0.55
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD11	10	0.55
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD12	10	0.55
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD13	10	0.55
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD11	1	0.55
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD12	1	0.55
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD13	1	0.55
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD21	1	0.55
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD22	1	0.55
(2,391)	1:39:A:CYS:SG	2:30:B:LEU:HD23	1	0.55
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD11	6	0.55
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD12	6	0.55
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD13	6	0.55
(1,166)	1:41:A:CYS:SG	1:91:A:MET:H	6	0.55
(6,67)	1:65:A:GLY:O	1:69:A:VAL:H	9	0.54
(5,9)	2:10:B:ALA:CA	2:11:B:ILE:CD1	2	0.54
(2,27)	1:39:A:CYS:SG	2:40:B:TYR:H	4	0.54
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD11	10	0.54
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD12	10	0.54
(1,425)	1:5:A:ILE:CG1	1:68:A:ILE:HD13	10	0.54
(6,156)	2:47:B:LEU:N	2:43:B:SER:O	2	0.53
(6,68)	1:69:A:VAL:N	1:65:A:GLY:O	4	0.53
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD11	3	0.53
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD12	3	0.53
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD13	3	0.53
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD11	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD12	2	0.53
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD13	2	0.53
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD11	10	0.53
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD12	10	0.53
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD13	10	0.53
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD11	4	0.53
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD12	4	0.53
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD13	4	0.53
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD21	4	0.53
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD22	4	0.53
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD23	4	0.53
(1,301)	2:39:B:CYS:SG	2:29:B:ARG:H	9	0.53
(1,220)	1:95:A:CYS:SG	1:90:A:GLY:H	7	0.53
(5,35)	2:28:B:THR:CB	2:30:B:LEU:CA	10	0.52
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD11	3	0.52
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD12	3	0.52
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD13	3	0.52
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD21	3	0.52
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD22	3	0.52
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD23	3	0.52
(1,284)	2:5:B:ILE:CG1	2:106:B:ARG:H	1	0.52
(6,156)	2:47:B:LEU:N	2:43:B:SER:O	10	0.51
(6,68)	1:69:A:VAL:N	1:65:A:GLY:O	9	0.51
(6,66)	1:68:A:ILE:N	1:64:A:SER:O	1	0.51
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD11	4	0.51
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD12	4	0.51
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD13	4	0.51
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD11	4	0.51
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD12	4	0.51
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD13	4	0.51
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD11	4	0.51
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD12	4	0.51
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD13	4	0.51
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD11	7	0.51
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD12	7	0.51
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD13	7	0.51
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD11	7	0.51
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD12	7	0.51
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD13	7	0.51
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD11	7	0.51
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD12	7	0.51
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD13	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD11	7	0.51
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD12	7	0.51
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD13	7	0.51
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD11	7	0.51
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD12	7	0.51
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD13	7	0.51
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD11	7	0.51
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD12	7	0.51
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD13	7	0.51
(2,39)	1:39:A:CYS:SG	2:62:B:ILE:H	2	0.51
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD11	4	0.51
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD12	4	0.51
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD13	4	0.51
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD21	4	0.51
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD22	4	0.51
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD23	4	0.51
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD11	2	0.51
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD12	2	0.51
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD13	2	0.51
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD21	2	0.51
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD22	2	0.51
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD23	2	0.51
(1,324)	2:39:B:CYS:SG	2:68:B:ILE:H	4	0.51
(1,180)	1:95:A:CYS:SG	1:10:A:ALA:H	3	0.51
(6,65)	1:64:A:SER:O	1:68:A:ILE:H	3	0.5
(1,351)	2:95:B:CYS:SG	2:6:B:TYR:H	9	0.5
(1,301)	2:39:B:CYS:SG	2:29:B:ARG:H	10	0.5
(1,296)	2:39:B:CYS:SG	2:24:B:SER:H	3	0.5
(1,166)	1:41:A:CYS:SG	1:91:A:MET:H	9	0.5
(5,35)	2:28:B:THR:CB	2:30:B:LEU:CA	7	0.49
(1,303)	2:39:B:CYS:SG	2:31:B:TRP:H	2	0.49
(1,284)	2:5:B:ILE:CG1	2:106:B:ARG:H	10	0.49
(6,66)	1:68:A:ILE:N	1:64:A:SER:O	3	0.48
(6,65)	1:64:A:SER:O	1:68:A:ILE:H	7	0.48
(6,28)	1:37:A:ILE:N	1:33:A:SER:O	6	0.48
(5,81)	1:43:A:SER:CA	1:45:A:TRP:CD2	10	0.48
(5,1)	1:93:A:LEU:CB	2:97:B:GLY:CA	2	0.48
(3,40)	2:63:B:TRP:CE2	2:66:B:VAL:CG1	2	0.48
(3,40)	2:63:B:TRP:CE2	2:66:B:VAL:CG2	2	0.48
(3,30)	2:89:B:ILE:HD11	1:100:A:ILE:HD11	3	0.48
(3,30)	2:89:B:ILE:HD11	1:100:A:ILE:HD12	3	0.48
(3,30)	2:89:B:ILE:HD11	1:100:A:ILE:HD13	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,30)	2:89:B:ILE:HD12	1:100:A:ILE:HD11	3	0.48
(3,30)	2:89:B:ILE:HD12	1:100:A:ILE:HD12	3	0.48
(3,30)	2:89:B:ILE:HD12	1:100:A:ILE:HD13	3	0.48
(3,30)	2:89:B:ILE:HD13	1:100:A:ILE:HD11	3	0.48
(3,30)	2:89:B:ILE:HD13	1:100:A:ILE:HD12	3	0.48
(3,30)	2:89:B:ILE:HD13	1:100:A:ILE:HD13	3	0.48
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD11	8	0.48
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD12	8	0.48
(3,27)	1:85:A:LEU:HD21	1:88:A:ILE:HD13	8	0.48
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD11	8	0.48
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD12	8	0.48
(3,27)	1:85:A:LEU:HD22	1:88:A:ILE:HD13	8	0.48
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD11	8	0.48
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD12	8	0.48
(3,27)	1:85:A:LEU:HD23	1:88:A:ILE:HD13	8	0.48
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD11	3	0.48
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD12	3	0.48
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD13	3	0.48
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD21	3	0.48
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD22	3	0.48
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD23	3	0.48
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD11	3	0.48
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD12	3	0.48
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD13	3	0.48
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD11	5	0.48
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD12	5	0.48
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD13	5	0.48
(2,27)	1:39:A:CYS:SG	2:40:B:TYR:H	6	0.48
(1,351)	2:95:B:CYS:SG	2:6:B:TYR:H	3	0.48
(1,220)	1:95:A:CYS:SG	1:90:A:GLY:H	6	0.48
(5,81)	1:43:A:SER:CA	1:45:A:TRP:CD2	6	0.47
(3,33)	1:47:A:LEU:HD11	3:201:A:P4P:H2B	1	0.47
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD11	5	0.47
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD12	5	0.47
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD13	5	0.47
(1,349)	2:95:B:CYS:SG	2:4:B:TYR:H	7	0.47
(5,81)	1:43:A:SER:CA	1:45:A:TRP:CD2	7	0.46
(5,7)	1:94:A:ILE:CB	2:97:B:GLY:CA	5	0.46
(1,369)	2:95:B:CYS:SG	2:40:B:TYR:H	6	0.46
(1,348)	2:95:B:CYS:SG	2:2:B:ASN:H	4	0.46
(1,219)	1:95:A:CYS:SG	1:89:A:ILE:H	8	0.46
(1,73)	1:39:A:CYS:SG	1:26:A:GLY:H	7	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,66)	1:68:A:ILE:N	1:64:A:SER:O	7	0.45
(5,35)	2:28:B:THR:CB	2:30:B:LEU:CA	8	0.45
(5,9)	2:10:B:ALA:CA	2:11:B:ILE:CD1	10	0.45
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD11	9	0.45
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD12	9	0.45
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD13	9	0.45
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD21	9	0.45
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD22	9	0.45
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD23	9	0.45
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD11	9	0.45
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD12	9	0.45
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD13	9	0.45
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD21	9	0.45
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD22	9	0.45
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD23	9	0.45
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD11	9	0.45
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD12	9	0.45
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD13	9	0.45
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD21	9	0.45
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD22	9	0.45
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD23	9	0.45
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD11	7	0.45
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD12	7	0.45
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD13	7	0.45
(2,27)	1:39:A:CYS:SG	2:40:B:TYR:H	9	0.45
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD11	7	0.45
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD12	7	0.45
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD13	7	0.45
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD21	7	0.45
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD22	7	0.45
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD23	7	0.45
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD11	4	0.45
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD12	4	0.45
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD13	4	0.45
(1,298)	2:39:B:CYS:SG	2:26:B:GLY:H	10	0.45
(6,67)	1:65:A:GLY:O	1:69:A:VAL:H	7	0.44
(5,95)	1:63:A:TRP:CA	1:14:A:GLU:CD	5	0.44
(5,5)	2:90:B:GLY:CA	1:97:A:GLY:CA	10	0.44
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD11	9	0.44
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD12	9	0.44
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD13	9	0.44
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD11	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD12	9	0.44
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD13	9	0.44
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD11	9	0.44
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD12	9	0.44
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD13	9	0.44
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD11	9	0.44
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD12	9	0.44
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD13	9	0.44
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD11	9	0.44
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD12	9	0.44
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD13	9	0.44
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD11	9	0.44
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD12	9	0.44
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD13	9	0.44
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD11	3	0.44
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD12	3	0.44
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD13	3	0.44
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD11	3	0.44
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD12	3	0.44
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD13	3	0.44
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD11	3	0.44
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD12	3	0.44
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD13	3	0.44
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD11	3	0.44
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD12	3	0.44
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD13	3	0.44
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD11	3	0.44
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD12	3	0.44
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD13	3	0.44
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD11	3	0.44
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD12	3	0.44
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD13	3	0.44
(2,27)	1:39:A:CYS:SG	2:40:B:TYR:H	1	0.44
(1,348)	2:95:B:CYS:SG	2:2:B:ASN:H	7	0.44
(1,303)	2:39:B:CYS:SG	2:31:B:TRP:H	6	0.44
(1,284)	2:5:B:ILE:CG1	2:106:B:ARG:H	2	0.44
(3,26)	1:85:A:LEU:HD11	1:88:A:ILE:HD11	1	0.43
(3,26)	1:85:A:LEU:HD11	1:88:A:ILE:HD12	1	0.43
(3,26)	1:85:A:LEU:HD11	1:88:A:ILE:HD13	1	0.43
(3,26)	1:85:A:LEU:HD12	1:88:A:ILE:HD11	1	0.43
(3,26)	1:85:A:LEU:HD12	1:88:A:ILE:HD12	1	0.43
(3,26)	1:85:A:LEU:HD12	1:88:A:ILE:HD13	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,26)	1:85:A:LEU:HD13	1:88:A:ILE:HD11	1	0.43
(3,26)	1:85:A:LEU:HD13	1:88:A:ILE:HD12	1	0.43
(3,26)	1:85:A:LEU:HD13	1:88:A:ILE:HD13	1	0.43
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD11	10	0.43
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD12	10	0.43
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD13	10	0.43
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD21	10	0.43
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD22	10	0.43
(3,15)	1:58:A:ILE:HD11	1:103:A:LEU:HD23	10	0.43
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD11	10	0.43
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD12	10	0.43
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD13	10	0.43
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD21	10	0.43
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD22	10	0.43
(3,15)	1:58:A:ILE:HD12	1:103:A:LEU:HD23	10	0.43
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD11	10	0.43
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD12	10	0.43
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD13	10	0.43
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD21	10	0.43
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD22	10	0.43
(3,15)	1:58:A:ILE:HD13	1:103:A:LEU:HD23	10	0.43
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD11	5	0.43
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD12	5	0.43
(3,6)	2:54:B:ILE:HD11	2:62:B:ILE:HD13	5	0.43
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD11	5	0.43
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD12	5	0.43
(3,6)	2:54:B:ILE:HD12	2:62:B:ILE:HD13	5	0.43
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD11	5	0.43
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD12	5	0.43
(3,6)	2:54:B:ILE:HD13	2:62:B:ILE:HD13	5	0.43
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD11	4	0.43
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD12	4	0.43
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD13	4	0.43
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD11	10	0.43
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD12	10	0.43
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD13	10	0.43
(2,40)	1:39:A:CYS:SG	2:63:B:TRP:H	2	0.43
(2,39)	1:39:A:CYS:SG	2:62:B:ILE:H	10	0.43
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD11	6	0.43
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD12	6	0.43
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD13	6	0.43
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD21	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD22	6	0.43
(1,515)	2:5:B:ILE:CG1	2:93:B:LEU:HD23	6	0.43
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD11	4	0.43
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD12	4	0.43
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD13	4	0.43
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD11	3	0.43
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD12	3	0.43
(1,483)	1:95:A:CYS:SG	1:16:A:ILE:HD13	3	0.43
(1,320)	2:39:B:CYS:SG	2:64:B:SER:H	6	0.43
(1,283)	2:5:B:ILE:CG1	2:105:B:SER:H	3	0.43
(1,219)	1:95:A:CYS:SG	1:89:A:ILE:H	1	0.43
(6,68)	1:69:A:VAL:N	1:65:A:GLY:O	7	0.42
(6,67)	1:65:A:GLY:O	1:69:A:VAL:H	6	0.42
(5,95)	1:63:A:TRP:CA	1:14:A:GLU:CD	6	0.42
(5,35)	2:28:B:THR:CB	2:30:B:LEU:CA	9	0.42
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD11	4	0.42
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD12	4	0.42
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD13	4	0.42
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD11	4	0.42
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD12	4	0.42
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD13	4	0.42
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD11	4	0.42
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD12	4	0.42
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD13	4	0.42
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD11	4	0.42
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD12	4	0.42
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD13	4	0.42
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD11	4	0.42
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD12	4	0.42
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD13	4	0.42
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD11	4	0.42
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD12	4	0.42
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD13	4	0.42
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD11	9	0.42
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD12	9	0.42
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD13	9	0.42
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD21	9	0.42
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD22	9	0.42
(2,389)	1:39:A:CYS:SG	2:7:B:LEU:HD23	9	0.42
(1,220)	1:95:A:CYS:SG	1:90:A:GLY:H	3	0.42
(1,198)	1:95:A:CYS:SG	1:54:A:ILE:H	7	0.42
(6,101)	1:95:A:CYS:O	1:99:A:LEU:H	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,27)	1:33:A:SER:O	1:37:A:ILE:H	7	0.41
(5,81)	1:43:A:SER:CA	1:45:A:TRP:CD2	8	0.41
(5,5)	2:90:B:GLY:CA	1:97:A:GLY:CA	7	0.41
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD11	8	0.41
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD12	8	0.41
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD13	8	0.41
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD11	8	0.41
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD12	8	0.41
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD13	8	0.41
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD11	8	0.41
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD12	8	0.41
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD13	8	0.41
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD11	8	0.41
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD12	8	0.41
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD13	8	0.41
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD11	8	0.41
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD12	8	0.41
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD13	8	0.41
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD11	8	0.41
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD12	8	0.41
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD13	8	0.41
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD11	9	0.41
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD12	9	0.41
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD13	9	0.41
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD11	9	0.41
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD12	9	0.41
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD13	9	0.41
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD11	9	0.41
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD12	9	0.41
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD13	9	0.41
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD11	9	0.41
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD12	9	0.41
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD13	9	0.41
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD11	9	0.41
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD12	9	0.41
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD13	9	0.41
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD11	9	0.41
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD12	9	0.41
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD13	9	0.41
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD11	4	0.41
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD12	4	0.41
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD13	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD11	4	0.41
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD12	4	0.41
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD13	4	0.41
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD11	4	0.41
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD12	4	0.41
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD13	4	0.41
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD11	4	0.41
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD12	4	0.41
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD13	4	0.41
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD11	4	0.41
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD12	4	0.41
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD13	4	0.41
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD11	4	0.41
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD12	4	0.41
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD13	4	0.41
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD11	10	0.41
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD12	10	0.41
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD13	10	0.41
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD11	10	0.41
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD12	10	0.41
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD13	10	0.41
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD11	10	0.41
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD12	10	0.41
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD13	10	0.41
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD11	10	0.41
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD12	10	0.41
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD13	10	0.41
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD11	10	0.41
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD12	10	0.41
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD13	10	0.41
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD11	10	0.41
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD12	10	0.41
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD13	10	0.41
(2,209)	2:39:B:CYS:SG	1:44:A:PHE:H	6	0.41
(2,30)	1:39:A:CYS:SG	2:51:B:LEU:H	4	0.41
(2,28)	1:39:A:CYS:SG	2:43:B:SER:H	4	0.41
(2,2)	2:39:B:CYS:SG	2:1:B:MET:HA	2	0.41
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD11	9	0.41
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD12	9	0.41
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD13	9	0.41
(1,370)	2:95:B:CYS:SG	2:43:B:SER:H	1	0.41
(1,351)	2:95:B:CYS:SG	2:6:B:TYR:H	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	2:5:B:ILE:CG1	2:105:B:SER:H	9	0.41
(1,177)	1:95:A:CYS:SG	1:7:A:LEU:H	7	0.41
(6,102)	1:99:A:LEU:N	1:95:A:CYS:O	6	0.4
(6,27)	1:33:A:SER:O	1:37:A:ILE:H	3	0.4
(5,81)	1:43:A:SER:CA	1:45:A:TRP:CD2	2	0.4
(5,35)	2:28:B:THR:CB	2:30:B:LEU:CA	2	0.4
(5,6)	1:90:A:GLY:CA	2:97:B:GLY:CA	2	0.4
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD11	9	0.4
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD12	9	0.4
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD13	9	0.4
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD11	9	0.4
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD12	9	0.4
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD13	9	0.4
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD11	9	0.4
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD12	9	0.4
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD13	9	0.4
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD11	9	0.4
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD12	9	0.4
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD13	9	0.4
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD11	9	0.4
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD12	9	0.4
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD13	9	0.4
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD11	9	0.4
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD12	9	0.4
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD13	9	0.4
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD11	9	0.4
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD12	9	0.4
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD13	9	0.4
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD11	9	0.4
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD12	9	0.4
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD13	9	0.4
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD11	9	0.4
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD12	9	0.4
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD13	9	0.4
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD11	9	0.4
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD12	9	0.4
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD13	9	0.4
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD11	9	0.4
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD12	9	0.4
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD13	9	0.4
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD11	9	0.4
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD12	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD13	9	0.4
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD11	9	0.4
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD12	9	0.4
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD13	9	0.4
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD21	9	0.4
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD22	9	0.4
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD23	9	0.4
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD11	9	0.4
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD12	9	0.4
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD13	9	0.4
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD21	9	0.4
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD22	9	0.4
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD23	9	0.4
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD11	9	0.4
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD12	9	0.4
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD13	9	0.4
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD21	9	0.4
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD22	9	0.4
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD23	9	0.4
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD11	6	0.4
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD12	6	0.4
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD13	6	0.4
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD21	6	0.4
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD22	6	0.4
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD23	6	0.4
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD11	1	0.4
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD12	1	0.4
(1,521)	2:39:B:CYS:SG	2:11:B:ILE:HD13	1	0.4
(1,369)	2:95:B:CYS:SG	2:40:B:TYR:H	5	0.4
(1,348)	2:95:B:CYS:SG	2:2:B:ASN:H	5	0.4
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD11	1	0.39
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD12	1	0.39
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD13	1	0.39
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD11	1	0.39
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD12	1	0.39
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD13	1	0.39
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD11	1	0.39
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD12	1	0.39
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD13	1	0.39
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD11	1	0.39
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD12	1	0.39
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD13	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD11	1	0.39
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD12	1	0.39
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD13	1	0.39
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD11	1	0.39
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD12	1	0.39
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD13	1	0.39
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD11	6	0.39
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD12	6	0.39
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD13	6	0.39
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD11	6	0.39
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD12	6	0.39
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD13	6	0.39
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD11	6	0.39
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD12	6	0.39
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD13	6	0.39
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD11	6	0.39
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD12	6	0.39
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD13	6	0.39
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD11	6	0.39
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD12	6	0.39
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD13	6	0.39
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD11	6	0.39
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD12	6	0.39
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD13	6	0.39
(2,421)	1:41:A:CYS:SG	2:101:B:ILE:HD11	10	0.39
(2,421)	1:41:A:CYS:SG	2:101:B:ILE:HD12	10	0.39
(2,421)	1:41:A:CYS:SG	2:101:B:ILE:HD13	10	0.39
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD11	7	0.39
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD12	7	0.39
(1,447)	1:39:A:CYS:SG	1:68:A:ILE:HD13	7	0.39
(1,303)	2:39:B:CYS:SG	2:31:B:TRP:H	9	0.39
(6,68)	1:69:A:VAL:N	1:65:A:GLY:O	6	0.38
(6,27)	1:33:A:SER:O	1:37:A:ILE:H	10	0.38
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD11	1	0.38
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD12	1	0.38
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD13	1	0.38
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD11	1	0.38
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD12	1	0.38
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD13	1	0.38
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD11	1	0.38
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD12	1	0.38
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD13	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD11	1	0.38
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD12	1	0.38
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD13	1	0.38
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD11	1	0.38
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD12	1	0.38
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD13	1	0.38
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD11	1	0.38
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD12	1	0.38
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD13	1	0.38
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD11	9	0.38
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD12	9	0.38
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD13	9	0.38
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD11	9	0.38
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD12	9	0.38
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD13	9	0.38
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD11	9	0.38
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD12	9	0.38
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD13	9	0.38
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD11	9	0.38
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD12	9	0.38
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD13	9	0.38
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD11	9	0.38
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD12	9	0.38
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD13	9	0.38
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD11	9	0.38
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD12	9	0.38
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD13	9	0.38
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD11	9	0.38
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD12	9	0.38
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD13	9	0.38
(6,154)	2:46:B:LEU:N	2:42:B:ALA:O	2	0.37
(6,113)	2:7:B:LEU:O	2:11:B:ILE:H	10	0.37
(6,65)	1:64:A:SER:O	1:68:A:ILE:H	4	0.37
(6,5)	1:7:A:LEU:O	1:11:A:ILE:H	7	0.37
(5,35)	2:28:B:THR:CB	2:30:B:LEU:CA	6	0.37
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD11	6	0.37
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD12	6	0.37
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD13	6	0.37
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD21	6	0.37
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD22	6	0.37
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD23	6	0.37
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD11	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD12	6	0.37
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD13	6	0.37
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD21	6	0.37
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD22	6	0.37
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD23	6	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD11	6	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD12	6	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD13	6	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD21	6	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD22	6	0.37
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD23	6	0.37
(3,11)	2:68:B:ILE:HD11	2:71:B:ILE:HD11	3	0.37
(3,11)	2:68:B:ILE:HD11	2:71:B:ILE:HD12	3	0.37
(3,11)	2:68:B:ILE:HD11	2:71:B:ILE:HD13	3	0.37
(3,11)	2:68:B:ILE:HD12	2:71:B:ILE:HD11	3	0.37
(3,11)	2:68:B:ILE:HD12	2:71:B:ILE:HD12	3	0.37
(3,11)	2:68:B:ILE:HD12	2:71:B:ILE:HD13	3	0.37
(3,11)	2:68:B:ILE:HD13	2:71:B:ILE:HD11	3	0.37
(3,11)	2:68:B:ILE:HD13	2:71:B:ILE:HD12	3	0.37
(3,11)	2:68:B:ILE:HD13	2:71:B:ILE:HD13	3	0.37
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD11	8	0.37
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD12	8	0.37
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD13	8	0.37
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD11	8	0.37
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD12	8	0.37
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD13	8	0.37
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD11	8	0.37
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD12	8	0.37
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD13	8	0.37
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD11	8	0.37
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD12	8	0.37
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD13	8	0.37
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD11	8	0.37
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD12	8	0.37
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD13	8	0.37
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD11	8	0.37
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD12	8	0.37
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD13	8	0.37
(2,28)	1:39:A:CYS:SG	2:43:B:SER:H	1	0.37
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD11	6	0.37
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD12	6	0.37
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD13	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD21	6	0.37
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD22	6	0.37
(1,550)	2:95:B:CYS:SG	2:74:B:LEU:HD23	6	0.37
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD11	8	0.37
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD12	8	0.37
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD13	8	0.37
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD21	8	0.37
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD22	8	0.37
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD23	8	0.37
(1,369)	2:95:B:CYS:SG	2:40:B:TYR:H	9	0.37
(1,348)	2:95:B:CYS:SG	2:2:B:ASN:H	6	0.37
(1,303)	2:39:B:CYS:SG	2:31:B:TRP:H	7	0.37
(1,301)	2:39:B:CYS:SG	2:29:B:ARG:H	2	0.37
(1,284)	2:5:B:ILE:CG1	2:106:B:ARG:H	9	0.37
(6,29)	1:34:A:VAL:O	1:38:A:ILE:H	10	0.36
(4,1)	1:14:A:GLU:OE1	2:60:B:TYR:OH	9	0.36
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD11	7	0.36
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD12	7	0.36
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD13	7	0.36
(2,37)	1:39:A:CYS:SG	2:59:B:ALA:H	8	0.36
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD11	8	0.36
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD12	8	0.36
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD13	8	0.36
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD21	8	0.36
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD22	8	0.36
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD23	8	0.36
(6,29)	1:34:A:VAL:O	1:38:A:ILE:H	3	0.35
(6,6)	1:11:A:ILE:N	1:7:A:LEU:O	7	0.35
(5,95)	1:63:A:TRP:CA	1:14:A:GLU:CD	10	0.35
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD11	1	0.35
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD12	1	0.35
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD13	1	0.35
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD11	1	0.35
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD12	1	0.35
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD13	1	0.35
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD11	1	0.35
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD12	1	0.35
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD13	1	0.35
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD11	1	0.35
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD12	1	0.35
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD13	1	0.35
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD11	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD12	1	0.35
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD13	1	0.35
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD11	1	0.35
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD12	1	0.35
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD13	1	0.35
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD11	6	0.35
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD12	6	0.35
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD13	6	0.35
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD11	6	0.35
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD12	6	0.35
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD13	6	0.35
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD11	6	0.35
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD12	6	0.35
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD13	6	0.35
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD11	6	0.35
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD12	6	0.35
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD13	6	0.35
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD11	6	0.35
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD12	6	0.35
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD13	6	0.35
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD11	6	0.35
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD12	6	0.35
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD13	6	0.35
(2,102)	1:41:A:CYS:SG	2:57:B:GLY:H	10	0.35
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD11	5	0.35
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD12	5	0.35
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD13	5	0.35
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD21	5	0.35
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD22	5	0.35
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD23	5	0.35
(6,30)	1:38:A:ILE:N	1:34:A:VAL:O	10	0.34
(6,28)	1:37:A:ILE:N	1:33:A:SER:O	7	0.34
(6,28)	1:37:A:ILE:N	1:33:A:SER:O	10	0.34
(5,95)	1:63:A:TRP:CA	1:14:A:GLU:CD	7	0.34
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD11	4	0.34
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD12	4	0.34
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD13	4	0.34
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD21	4	0.34
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD22	4	0.34
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD23	4	0.34
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD11	4	0.34
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD12	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD13	4	0.34
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD21	4	0.34
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD22	4	0.34
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD23	4	0.34
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD11	4	0.34
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD12	4	0.34
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD13	4	0.34
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD21	4	0.34
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD22	4	0.34
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD23	4	0.34
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD11	7	0.34
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD12	7	0.34
(2,449)	2:41:B:CYS:SG	1:68:A:ILE:HD13	7	0.34
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD11	2	0.34
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD12	2	0.34
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD13	2	0.34
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD11	1	0.34
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD12	1	0.34
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD13	1	0.34
(1,470)	1:41:A:CYS:SG	1:68:A:ILE:HD11	5	0.34
(1,470)	1:41:A:CYS:SG	1:68:A:ILE:HD12	5	0.34
(1,470)	1:41:A:CYS:SG	1:68:A:ILE:HD13	5	0.34
(1,320)	2:39:B:CYS:SG	2:64:B:SER:H	10	0.34
(1,199)	1:95:A:CYS:SG	1:57:A:GLY:H	2	0.34
(5,95)	1:63:A:TRP:CA	1:14:A:GLU:CD	2	0.33
(5,95)	1:63:A:TRP:CA	1:14:A:GLU:CD	3	0.33
(5,2)	1:93:A:LEU:CG	2:97:B:GLY:CA	4	0.33
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD11	9	0.33
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD12	9	0.33
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD13	9	0.33
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD11	9	0.33
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD12	9	0.33
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD13	9	0.33
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD11	9	0.33
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD12	9	0.33
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD13	9	0.33
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD11	9	0.33
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD12	9	0.33
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD13	9	0.33
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD11	9	0.33
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD12	9	0.33
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD13	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD11	9	0.33
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD12	9	0.33
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD13	9	0.33
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD11	10	0.33
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD12	10	0.33
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD13	10	0.33
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD21	10	0.33
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD22	10	0.33
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD23	10	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD11	10	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD12	10	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD13	10	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD21	10	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD22	10	0.33
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD23	10	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD11	10	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD12	10	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD13	10	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD21	10	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD22	10	0.33
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD23	10	0.33
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD11	5	0.33
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD12	5	0.33
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD13	5	0.33
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD11	5	0.33
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD12	5	0.33
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD13	5	0.33
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD11	5	0.33
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD12	5	0.33
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD13	5	0.33
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD11	5	0.33
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD12	5	0.33
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD13	5	0.33
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD11	5	0.33
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD12	5	0.33
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD13	5	0.33
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD11	5	0.33
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD12	5	0.33
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD13	5	0.33
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD11	7	0.33
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD12	7	0.33
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD13	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD21	7	0.33
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD22	7	0.33
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD23	7	0.33
(1,166)	1:41:A:CYS:SG	1:91:A:MET:H	4	0.33
(6,66)	1:68:A:ILE:N	1:64:A:SER:O	4	0.32
(6,28)	1:37:A:ILE:N	1:33:A:SER:O	3	0.32
(3,33)	1:47:A:LEU:HD11	3:201:A:P4P:H2A	2	0.32
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD11	5	0.32
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD12	5	0.32
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD13	5	0.32
(2,39)	1:39:A:CYS:SG	2:62:B:ILE:H	7	0.32
(6,30)	1:38:A:ILE:N	1:34:A:VAL:O	3	0.31
(6,27)	1:33:A:SER:O	1:37:A:ILE:H	4	0.31
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD11	5	0.31
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD12	5	0.31
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD13	5	0.31
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD21	5	0.31
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD22	5	0.31
(3,14)	2:89:B:ILE:HD11	2:85:B:LEU:HD23	5	0.31
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD11	5	0.31
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD12	5	0.31
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD13	5	0.31
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD21	5	0.31
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD22	5	0.31
(3,14)	2:89:B:ILE:HD12	2:85:B:LEU:HD23	5	0.31
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD11	5	0.31
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD12	5	0.31
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD13	5	0.31
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD21	5	0.31
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD22	5	0.31
(3,14)	2:89:B:ILE:HD13	2:85:B:LEU:HD23	5	0.31
(2,41)	1:39:A:CYS:SG	2:64:B:SER:H	8	0.31
(2,40)	1:39:A:CYS:SG	2:63:B:TRP:H	10	0.31
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD11	3	0.31
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD12	3	0.31
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD13	3	0.31
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD11	1	0.31
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD12	1	0.31
(1,517)	2:5:B:ILE:CG1	2:100:B:ILE:HD13	1	0.31
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD11	2	0.31
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD12	2	0.31
(1,501)	2:5:B:ILE:CG1	2:11:B:ILE:HD13	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	2:95:B:CYS:SG	2:43:B:SER:H	8	0.31
(1,179)	1:95:A:CYS:SG	1:9:A:GLY:H	3	0.31
(6,27)	1:33:A:SER:O	1:37:A:ILE:H	2	0.3
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD11	10	0.3
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD12	10	0.3
(3,19)	1:7:A:LEU:HD11	1:54:A:ILE:HD13	10	0.3
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD11	10	0.3
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD12	10	0.3
(3,19)	1:7:A:LEU:HD12	1:54:A:ILE:HD13	10	0.3
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD11	10	0.3
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD12	10	0.3
(3,19)	1:7:A:LEU:HD13	1:54:A:ILE:HD13	10	0.3
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD11	10	0.3
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD12	10	0.3
(3,19)	1:7:A:LEU:HD21	1:54:A:ILE:HD13	10	0.3
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD11	10	0.3
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD12	10	0.3
(3,19)	1:7:A:LEU:HD22	1:54:A:ILE:HD13	10	0.3
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD11	10	0.3
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD12	10	0.3
(3,19)	1:7:A:LEU:HD23	1:54:A:ILE:HD13	10	0.3
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD11	2	0.3
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD12	2	0.3
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD13	2	0.3
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD11	2	0.3
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD12	2	0.3
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD13	2	0.3
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD11	2	0.3
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD12	2	0.3
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD13	2	0.3
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD11	2	0.3
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD12	2	0.3
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD13	2	0.3
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD11	2	0.3
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD12	2	0.3
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD13	2	0.3
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD11	2	0.3
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD12	2	0.3
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD13	2	0.3
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD11	5	0.3
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD12	5	0.3
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD13	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD11	5	0.3
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD12	5	0.3
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD13	5	0.3
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD11	5	0.3
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD12	5	0.3
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD13	5	0.3
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD11	5	0.3
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD12	5	0.3
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD13	5	0.3
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD11	5	0.3
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD12	5	0.3
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD13	5	0.3
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD11	5	0.3
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD12	5	0.3
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD13	5	0.3
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD11	10	0.3
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD12	10	0.3
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD13	10	0.3
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD11	8	0.3
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD12	8	0.3
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD13	8	0.3
(2,158)	2:30:B:LEU:CG	1:45:A:TRP:H	4	0.3
(2,158)	2:30:B:LEU:CG	1:45:A:TRP:H	8	0.3
(2,102)	1:41:A:CYS:SG	2:57:B:GLY:H	6	0.3
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD11	1	0.3
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD12	1	0.3
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD13	1	0.3
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD21	1	0.3
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD22	1	0.3
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD23	1	0.3
(6,114)	2:11:B:ILE:N	2:7:B:LEU:O	10	0.29
(5,7)	1:94:A:ILE:CB	2:97:B:GLY:CA	10	0.29
(5,1)	1:93:A:LEU:CB	2:97:B:GLY:CA	5	0.29
(3,33)	1:47:A:LEU:HD11	3:201:A:P4P:H2B	3	0.29
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD11	3	0.29
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD12	3	0.29
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD13	3	0.29
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD21	3	0.29
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD22	3	0.29
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD23	3	0.29
(1,283)	2:5:B:ILE:CG1	2:105:B:SER:H	7	0.29
(1,166)	1:41:A:CYS:SG	1:91:A:MET:H	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,40)	2:63:B:TRP:CE2	2:66:B:VAL:CG1	4	0.28
(3,40)	2:63:B:TRP:CE2	2:66:B:VAL:CG2	4	0.28
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD11	6	0.28
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD12	6	0.28
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD13	6	0.28
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD11	6	0.28
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD12	6	0.28
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD13	6	0.28
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD11	6	0.28
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD12	6	0.28
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD13	6	0.28
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD11	6	0.28
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD12	6	0.28
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD13	6	0.28
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD11	6	0.28
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD12	6	0.28
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD13	6	0.28
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD11	6	0.28
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD12	6	0.28
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD13	6	0.28
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD11	7	0.28
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD12	7	0.28
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD13	7	0.28
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD21	7	0.28
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD22	7	0.28
(3,13)	2:88:B:ILE:HD11	2:83:B:LEU:HD23	7	0.28
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD11	7	0.28
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD12	7	0.28
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD13	7	0.28
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD21	7	0.28
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD22	7	0.28
(3,13)	2:88:B:ILE:HD12	2:83:B:LEU:HD23	7	0.28
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD11	7	0.28
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD12	7	0.28
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD13	7	0.28
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD21	7	0.28
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD22	7	0.28
(3,13)	2:88:B:ILE:HD13	2:83:B:LEU:HD23	7	0.28
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD11	6	0.28
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD12	6	0.28
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD13	6	0.28
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD11	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD12	6	0.28
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD13	6	0.28
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD11	6	0.28
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD12	6	0.28
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD13	6	0.28
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD11	6	0.28
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD12	6	0.28
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD13	6	0.28
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD11	6	0.28
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD12	6	0.28
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD13	6	0.28
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD11	6	0.28
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD12	6	0.28
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD13	6	0.28
(2,114)	1:41:A:CYS:SG	2:70:B:LEU:H	8	0.28
(1,369)	2:95:B:CYS:SG	2:40:B:TYR:H	2	0.28
(1,284)	2:5:B:ILE:CG1	2:106:B:ARG:H	8	0.28
(1,220)	1:95:A:CYS:SG	1:90:A:GLY:H	9	0.28
(6,29)	1:34:A:VAL:O	1:38:A:ILE:H	6	0.27
(5,95)	1:63:A:TRP:CA	1:14:A:GLU:CD	4	0.27
(5,35)	2:28:B:THR:CB	2:30:B:LEU:CA	4	0.27
(5,9)	2:10:B:ALA:CA	2:11:B:ILE:CD1	4	0.27
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD11	1	0.27
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD12	1	0.27
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD13	1	0.27
(2,114)	1:41:A:CYS:SG	2:70:B:LEU:H	3	0.27
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD11	6	0.27
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD12	6	0.27
(1,516)	2:5:B:ILE:CG1	2:94:B:ILE:HD13	6	0.27
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD11	1	0.27
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD12	1	0.27
(1,499)	1:95:A:CYS:SG	1:101:A:ILE:HD13	1	0.27
(6,155)	2:43:B:SER:O	2:47:B:LEU:H	1	0.26
(6,29)	1:34:A:VAL:O	1:38:A:ILE:H	7	0.26
(3,30)	2:89:B:ILE:HD11	1:100:A:ILE:HD11	4	0.26
(3,30)	2:89:B:ILE:HD11	1:100:A:ILE:HD12	4	0.26
(3,30)	2:89:B:ILE:HD11	1:100:A:ILE:HD13	4	0.26
(3,30)	2:89:B:ILE:HD12	1:100:A:ILE:HD11	4	0.26
(3,30)	2:89:B:ILE:HD12	1:100:A:ILE:HD12	4	0.26
(3,30)	2:89:B:ILE:HD12	1:100:A:ILE:HD13	4	0.26
(3,30)	2:89:B:ILE:HD13	1:100:A:ILE:HD11	4	0.26
(3,30)	2:89:B:ILE:HD13	1:100:A:ILE:HD12	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,30)	2:89:B:ILE:HD13	1:100:A:ILE:HD13	4	0.26
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD11	6	0.26
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD12	6	0.26
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD13	6	0.26
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD11	6	0.26
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD12	6	0.26
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD13	6	0.26
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD11	6	0.26
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD12	6	0.26
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD13	6	0.26
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD11	6	0.26
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD12	6	0.26
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD13	6	0.26
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD11	6	0.26
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD12	6	0.26
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD13	6	0.26
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD11	6	0.26
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD12	6	0.26
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD13	6	0.26
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD11	3	0.26
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD12	3	0.26
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD13	3	0.26
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD11	3	0.26
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD12	3	0.26
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD13	3	0.26
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD11	3	0.26
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD12	3	0.26
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD13	3	0.26
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD11	3	0.26
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD12	3	0.26
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD13	3	0.26
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD11	3	0.26
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD12	3	0.26
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD13	3	0.26
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD11	3	0.26
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD12	3	0.26
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD13	3	0.26
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG11	4	0.26
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG12	4	0.26
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG13	4	0.26
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG21	4	0.26
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG22	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG23	4	0.26
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG11	4	0.26
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG12	4	0.26
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG13	4	0.26
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG21	4	0.26
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG22	4	0.26
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG23	4	0.26
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG11	4	0.26
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG12	4	0.26
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG13	4	0.26
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG21	4	0.26
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG22	4	0.26
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG23	4	0.26
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD11	1	0.26
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD12	1	0.26
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD13	1	0.26
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD21	1	0.26
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD22	1	0.26
(1,534)	2:39:B:CYS:SG	2:93:B:LEU:HD23	1	0.26
(1,348)	2:95:B:CYS:SG	2:2:B:ASN:H	10	0.26
(1,303)	2:39:B:CYS:SG	2:31:B:TRP:H	10	0.26
(6,153)	2:42:B:ALA:O	2:46:B:LEU:H	10	0.25
(6,28)	1:37:A:ILE:N	1:33:A:SER:O	4	0.25
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD11	2	0.25
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD12	2	0.25
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD13	2	0.25
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD11	2	0.25
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD12	2	0.25
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD13	2	0.25
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD11	2	0.25
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD12	2	0.25
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD13	2	0.25
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD11	2	0.25
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD12	2	0.25
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD13	2	0.25
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD11	2	0.25
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD12	2	0.25
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD13	2	0.25
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD11	2	0.25
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD12	2	0.25
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD13	2	0.25
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD11	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD12	2	0.25
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD13	2	0.25
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD11	2	0.25
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD12	2	0.25
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD13	2	0.25
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD11	2	0.25
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD12	2	0.25
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD13	2	0.25
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD11	2	0.25
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD12	2	0.25
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD13	2	0.25
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD11	2	0.25
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD12	2	0.25
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD13	2	0.25
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD11	2	0.25
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD12	2	0.25
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD13	2	0.25
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD11	2	0.25
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD12	2	0.25
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD13	2	0.25
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD11	2	0.25
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD12	2	0.25
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD13	2	0.25
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD11	2	0.25
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD12	2	0.25
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD13	2	0.25
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD11	2	0.25
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD12	2	0.25
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD13	2	0.25
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD11	2	0.25
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD12	2	0.25
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD13	2	0.25
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD11	2	0.25
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD12	2	0.25
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD13	2	0.25
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG11	3	0.25
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG12	3	0.25
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG13	3	0.25
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG21	3	0.25
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG22	3	0.25
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG23	3	0.25
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG11	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG12	3	0.25
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG13	3	0.25
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG21	3	0.25
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG22	3	0.25
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG23	3	0.25
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG11	3	0.25
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG12	3	0.25
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG13	3	0.25
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG21	3	0.25
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG22	3	0.25
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG23	3	0.25
(6,28)	1:37:A:ILE:N	1:33:A:SER:O	2	0.24
(5,5)	2:90:B:GLY:CA	1:97:A:GLY:CA	5	0.24
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD11	9	0.24
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD12	9	0.24
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD13	9	0.24
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD11	5	0.24
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD12	5	0.24
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD13	5	0.24
(2,158)	2:30:B:LEU:CG	1:45:A:TRP:H	2	0.24
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD11	6	0.24
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD12	6	0.24
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD13	6	0.24
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD21	6	0.24
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD22	6	0.24
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD23	6	0.24
(5,81)	1:43:A:SER:CA	1:45:A:TRP:CD2	1	0.23
(3,39)	2:63:B:TRP:CE2	2:47:B:LEU:CD1	4	0.23
(3,39)	2:63:B:TRP:CE2	2:47:B:LEU:CD2	4	0.23
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD11	4	0.23
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD12	4	0.23
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD13	4	0.23
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD11	4	0.23
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD12	4	0.23
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD13	4	0.23
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD11	4	0.23
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD12	4	0.23
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD13	4	0.23
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD11	4	0.23
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD12	4	0.23
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD13	4	0.23
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD11	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD12	4	0.23
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD13	4	0.23
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD11	4	0.23
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD12	4	0.23
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD13	4	0.23
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD11	7	0.23
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD12	7	0.23
(3,5)	2:34:B:VAL:HG11	2:38:B:ILE:HD13	7	0.23
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD11	7	0.23
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD12	7	0.23
(3,5)	2:34:B:VAL:HG12	2:38:B:ILE:HD13	7	0.23
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD11	7	0.23
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD12	7	0.23
(3,5)	2:34:B:VAL:HG13	2:38:B:ILE:HD13	7	0.23
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD11	7	0.23
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD12	7	0.23
(3,5)	2:34:B:VAL:HG21	2:38:B:ILE:HD13	7	0.23
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD11	7	0.23
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD12	7	0.23
(3,5)	2:34:B:VAL:HG22	2:38:B:ILE:HD13	7	0.23
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD11	7	0.23
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD12	7	0.23
(3,5)	2:34:B:VAL:HG23	2:38:B:ILE:HD13	7	0.23
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD11	6	0.23
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD12	6	0.23
(2,395)	1:39:A:CYS:SG	2:62:B:ILE:HD13	6	0.23
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD11	9	0.23
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD12	9	0.23
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD13	9	0.23
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD21	9	0.23
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD22	9	0.23
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD23	9	0.23
(1,176)	1:95:A:CYS:SG	1:6:A:TYR:H	9	0.23
(6,99)	1:94:A:ILE:O	1:98:A:VAL:H	1	0.22
(6,69)	1:66:A:VAL:O	1:70:A:LEU:H	1	0.22
(6,30)	1:38:A:ILE:N	1:34:A:VAL:O	7	0.22
(5,81)	1:43:A:SER:CA	1:45:A:TRP:CD2	9	0.22
(5,11)	2:25:B:GLU:CD	2:22:B:LYS:CE	9	0.22
(4,1)	1:14:A:GLU:OE1	2:60:B:TYR:OH	1	0.22
(3,34)	1:47:A:LEU:HD12	3:201:A:P4P:H2A	8	0.22
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD11	8	0.22
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD12	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD13	8	0.22
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD11	8	0.22
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD12	8	0.22
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD13	8	0.22
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD11	8	0.22
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD12	8	0.22
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD13	8	0.22
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD11	8	0.22
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD12	8	0.22
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD13	8	0.22
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD11	8	0.22
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD12	8	0.22
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD13	8	0.22
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD11	8	0.22
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD12	8	0.22
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD13	8	0.22
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD11	10	0.22
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD12	10	0.22
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD13	10	0.22
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD11	10	0.22
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD12	10	0.22
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD13	10	0.22
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD11	10	0.22
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD12	10	0.22
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD13	10	0.22
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD11	10	0.22
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD12	10	0.22
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD13	10	0.22
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD11	10	0.22
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD12	10	0.22
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD13	10	0.22
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD11	10	0.22
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD12	10	0.22
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD13	10	0.22
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG11	6	0.22
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG12	6	0.22
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG13	6	0.22
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG21	6	0.22
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG22	6	0.22
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG23	6	0.22
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG11	6	0.22
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG12	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG13	6	0.22
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG21	6	0.22
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG22	6	0.22
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG23	6	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG11	6	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG12	6	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG13	6	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG21	6	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG22	6	0.22
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG23	6	0.22
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD11	4	0.22
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD12	4	0.22
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD13	4	0.22
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD21	4	0.22
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD22	4	0.22
(2,453)	2:41:B:CYS:SG	1:83:A:LEU:HD23	4	0.22
(2,102)	1:41:A:CYS:SG	2:57:B:GLY:H	1	0.22
(2,102)	1:41:A:CYS:SG	2:57:B:GLY:H	5	0.22
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD11	10	0.22
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD12	10	0.22
(1,476)	1:41:A:CYS:SG	1:16:A:ILE:HD13	10	0.22
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD11	10	0.22
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD12	10	0.22
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD13	10	0.22
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD21	10	0.22
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD22	10	0.22
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD23	10	0.22
(1,350)	2:95:B:CYS:SG	2:5:B:ILE:H	9	0.22
(6,30)	1:38:A:ILE:N	1:34:A:VAL:O	6	0.21
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD11	1	0.21
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD12	1	0.21
(3,18)	1:83:A:LEU:HD11	1:88:A:ILE:HD13	1	0.21
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD11	1	0.21
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD12	1	0.21
(3,18)	1:83:A:LEU:HD12	1:88:A:ILE:HD13	1	0.21
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD11	1	0.21
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD12	1	0.21
(3,18)	1:83:A:LEU:HD13	1:88:A:ILE:HD13	1	0.21
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD11	1	0.21
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD12	1	0.21
(3,18)	1:83:A:LEU:HD21	1:88:A:ILE:HD13	1	0.21
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD11	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD12	1	0.21
(3,18)	1:83:A:LEU:HD22	1:88:A:ILE:HD13	1	0.21
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD11	1	0.21
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD12	1	0.21
(3,18)	1:83:A:LEU:HD23	1:88:A:ILE:HD13	1	0.21
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD11	1	0.21
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD12	1	0.21
(3,16)	1:83:A:LEU:HD11	1:88:A:ILE:HD13	1	0.21
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD11	1	0.21
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD12	1	0.21
(3,16)	1:83:A:LEU:HD12	1:88:A:ILE:HD13	1	0.21
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD11	1	0.21
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD12	1	0.21
(3,16)	1:83:A:LEU:HD13	1:88:A:ILE:HD13	1	0.21
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD11	1	0.21
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD12	1	0.21
(3,16)	1:83:A:LEU:HD21	1:88:A:ILE:HD13	1	0.21
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD11	1	0.21
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD12	1	0.21
(3,16)	1:83:A:LEU:HD22	1:88:A:ILE:HD13	1	0.21
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD11	1	0.21
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD12	1	0.21
(3,16)	1:83:A:LEU:HD23	1:88:A:ILE:HD13	1	0.21
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD11	10	0.21
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD12	10	0.21
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD13	10	0.21
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD11	1	0.21
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD12	1	0.21
(2,441)	2:41:B:CYS:SG	1:11:A:ILE:HD13	1	0.21
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD11	6	0.21
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD12	6	0.21
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD13	6	0.21
(2,408)	1:41:A:CYS:SG	2:51:B:LEU:HD11	1	0.21
(2,408)	1:41:A:CYS:SG	2:51:B:LEU:HD12	1	0.21
(2,408)	1:41:A:CYS:SG	2:51:B:LEU:HD13	1	0.21
(2,408)	1:41:A:CYS:SG	2:51:B:LEU:HD21	1	0.21
(2,408)	1:41:A:CYS:SG	2:51:B:LEU:HD22	1	0.21
(2,408)	1:41:A:CYS:SG	2:51:B:LEU:HD23	1	0.21
(2,81)	1:41:A:CYS:SG	2:24:B:SER:H	3	0.21
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD11	4	0.21
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD12	4	0.21
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD13	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD21	4	0.21
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD22	4	0.21
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD23	4	0.21
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD11	6	0.21
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD12	6	0.21
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD13	6	0.21
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD21	6	0.21
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD22	6	0.21
(1,460)	1:41:A:CYS:SG	1:7:A:LEU:HD23	6	0.21
(1,351)	2:95:B:CYS:SG	2:6:B:TYR:H	1	0.21
(1,298)	2:39:B:CYS:SG	2:26:B:GLY:H	2	0.21
(1,201)	1:95:A:CYS:SG	1:60:A:TYR:H	4	0.21
(6,100)	1:98:A:VAL:N	1:94:A:ILE:O	1	0.2
(6,29)	1:34:A:VAL:O	1:38:A:ILE:H	4	0.2
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD11	4	0.2
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD12	4	0.2
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD13	4	0.2
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD11	4	0.2
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD12	4	0.2
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD13	4	0.2
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD11	4	0.2
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD12	4	0.2
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD13	4	0.2
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD11	4	0.2
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD12	4	0.2
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD13	4	0.2
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD11	4	0.2
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD12	4	0.2
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD13	4	0.2
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD11	4	0.2
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD12	4	0.2
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD13	4	0.2
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD11	10	0.2
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD12	10	0.2
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD13	10	0.2
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD11	10	0.2
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD12	10	0.2
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD13	10	0.2
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD11	10	0.2
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD12	10	0.2
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD13	10	0.2
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD11	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD12	10	0.2
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD13	10	0.2
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD11	10	0.2
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD12	10	0.2
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD13	10	0.2
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD11	10	0.2
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD12	10	0.2
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD13	10	0.2
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD11	2	0.2
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD12	2	0.2
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD13	2	0.2
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD21	2	0.2
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD22	2	0.2
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD23	2	0.2
(2,209)	2:39:B:CYS:SG	1:44:A:PHE:H	2	0.2
(1,526)	2:39:B:CYS:SG	2:58:B:ILE:HD11	4	0.2
(1,526)	2:39:B:CYS:SG	2:58:B:ILE:HD12	4	0.2
(1,526)	2:39:B:CYS:SG	2:58:B:ILE:HD13	4	0.2
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD11	6	0.2
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD12	6	0.2
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD13	6	0.2
(1,298)	2:39:B:CYS:SG	2:26:B:GLY:H	6	0.2
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD11	1	0.19
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD12	1	0.19
(3,1)	2:7:B:LEU:HD11	2:54:B:ILE:HD13	1	0.19
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD11	1	0.19
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD12	1	0.19
(3,1)	2:7:B:LEU:HD12	2:54:B:ILE:HD13	1	0.19
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD11	1	0.19
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD12	1	0.19
(3,1)	2:7:B:LEU:HD13	2:54:B:ILE:HD13	1	0.19
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD11	1	0.19
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD12	1	0.19
(3,1)	2:7:B:LEU:HD21	2:54:B:ILE:HD13	1	0.19
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD11	1	0.19
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD12	1	0.19
(3,1)	2:7:B:LEU:HD22	2:54:B:ILE:HD13	1	0.19
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD11	1	0.19
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD12	1	0.19
(3,1)	2:7:B:LEU:HD23	2:54:B:ILE:HD13	1	0.19
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD11	9	0.19
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD12	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,410)	1:41:A:CYS:SG	2:58:B:ILE:HD13	9	0.19
(6,70)	1:70:A:LEU:N	1:66:A:VAL:O	1	0.18
(5,72)	1:34:A:VAL:CA	1:31:A:TRP:CD2	9	0.18
(5,6)	1:90:A:GLY:CA	2:97:B:GLY:CA	1	0.18
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD11	7	0.18
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD12	7	0.18
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD13	7	0.18
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD11	7	0.18
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD12	7	0.18
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD13	7	0.18
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD11	7	0.18
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD12	7	0.18
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD13	7	0.18
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD11	7	0.18
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD12	7	0.18
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD13	7	0.18
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD11	7	0.18
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD12	7	0.18
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD13	7	0.18
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD11	7	0.18
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD12	7	0.18
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD13	7	0.18
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD11	10	0.18
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD12	10	0.18
(2,397)	1:39:A:CYS:SG	2:71:B:ILE:HD13	10	0.18
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD11	6	0.18
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD12	6	0.18
(1,475)	1:41:A:CYS:SG	1:88:A:ILE:HD13	6	0.18
(1,324)	2:39:B:CYS:SG	2:68:B:ILE:H	6	0.18
(1,320)	2:39:B:CYS:SG	2:64:B:SER:H	2	0.18
(1,298)	2:39:B:CYS:SG	2:26:B:GLY:H	8	0.18
(1,200)	1:95:A:CYS:SG	1:59:A:ALA:H	7	0.18
(1,199)	1:95:A:CYS:SG	1:57:A:GLY:H	3	0.18
(6,156)	2:47:B:LEU:N	2:43:B:SER:O	1	0.17
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD11	9	0.17
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD12	9	0.17
(3,10)	2:66:B:VAL:HG11	2:11:B:ILE:HD13	9	0.17
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD11	9	0.17
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD12	9	0.17
(3,10)	2:66:B:VAL:HG12	2:11:B:ILE:HD13	9	0.17
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD11	9	0.17
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD12	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,10)	2:66:B:VAL:HG13	2:11:B:ILE:HD13	9	0.17
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD11	9	0.17
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD12	9	0.17
(3,10)	2:66:B:VAL:HG21	2:11:B:ILE:HD13	9	0.17
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD11	9	0.17
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD12	9	0.17
(3,10)	2:66:B:VAL:HG22	2:11:B:ILE:HD13	9	0.17
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD11	9	0.17
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD12	9	0.17
(3,10)	2:66:B:VAL:HG23	2:11:B:ILE:HD13	9	0.17
(2,102)	1:41:A:CYS:SG	2:57:B:GLY:H	9	0.17
(2,40)	1:39:A:CYS:SG	2:63:B:TRP:H	7	0.17
(6,30)	1:38:A:ILE:N	1:34:A:VAL:O	4	0.16
(6,27)	1:33:A:SER:O	1:37:A:ILE:H	9	0.16
(5,11)	2:25:B:GLU:CD	2:22:B:LYS:CE	10	0.16
(3,39)	2:63:B:TRP:CE2	2:47:B:LEU:CD1	10	0.16
(3,39)	2:63:B:TRP:CE2	2:47:B:LEU:CD2	10	0.16
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD11	10	0.16
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD12	10	0.16
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD13	10	0.16
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD21	10	0.16
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD22	10	0.16
(3,17)	1:89:A:ILE:HD11	1:93:A:LEU:HD23	10	0.16
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD11	10	0.16
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD12	10	0.16
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD13	10	0.16
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD21	10	0.16
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD22	10	0.16
(3,17)	1:89:A:ILE:HD12	1:93:A:LEU:HD23	10	0.16
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD11	10	0.16
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD12	10	0.16
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD13	10	0.16
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD21	10	0.16
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD22	10	0.16
(3,17)	1:89:A:ILE:HD13	1:93:A:LEU:HD23	10	0.16
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD11	8	0.16
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD12	8	0.16
(3,12)	2:85:B:LEU:HD11	2:88:B:ILE:HD13	8	0.16
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD11	8	0.16
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD12	8	0.16
(3,12)	2:85:B:LEU:HD12	2:88:B:ILE:HD13	8	0.16
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD11	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD12	8	0.16
(3,12)	2:85:B:LEU:HD13	2:88:B:ILE:HD13	8	0.16
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD11	8	0.16
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD12	8	0.16
(3,12)	2:85:B:LEU:HD21	2:88:B:ILE:HD13	8	0.16
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD11	8	0.16
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD12	8	0.16
(3,12)	2:85:B:LEU:HD22	2:88:B:ILE:HD13	8	0.16
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD11	8	0.16
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD12	8	0.16
(3,12)	2:85:B:LEU:HD23	2:88:B:ILE:HD13	8	0.16
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD11	2	0.16
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD12	2	0.16
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD13	2	0.16
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD21	2	0.16
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD22	2	0.16
(1,524)	2:39:B:CYS:SG	2:51:B:LEU:HD23	2	0.16
(1,320)	2:39:B:CYS:SG	2:64:B:SER:H	5	0.16
(6,157)	2:44:B:PHE:O	2:48:B:ALA:H	10	0.15
(6,27)	1:33:A:SER:O	1:37:A:ILE:H	8	0.15
(5,95)	1:63:A:TRP:CA	1:14:A:GLU:CD	9	0.15
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD11	3	0.15
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD12	3	0.15
(3,25)	1:68:A:ILE:HD11	1:94:A:ILE:HD13	3	0.15
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD11	3	0.15
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD12	3	0.15
(3,25)	1:68:A:ILE:HD12	1:94:A:ILE:HD13	3	0.15
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD11	3	0.15
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD12	3	0.15
(3,25)	1:68:A:ILE:HD13	1:94:A:ILE:HD13	3	0.15
(1,320)	2:39:B:CYS:SG	2:64:B:SER:H	3	0.15
(5,6)	1:90:A:GLY:CA	2:97:B:GLY:CA	6	0.14
(3,28)	1:85:A:LEU:HD11	1:89:A:ILE:HD11	6	0.14
(3,28)	1:85:A:LEU:HD11	1:89:A:ILE:HD12	6	0.14
(3,28)	1:85:A:LEU:HD11	1:89:A:ILE:HD13	6	0.14
(3,28)	1:85:A:LEU:HD12	1:89:A:ILE:HD11	6	0.14
(3,28)	1:85:A:LEU:HD12	1:89:A:ILE:HD12	6	0.14
(3,28)	1:85:A:LEU:HD12	1:89:A:ILE:HD13	6	0.14
(3,28)	1:85:A:LEU:HD13	1:89:A:ILE:HD11	6	0.14
(3,28)	1:85:A:LEU:HD13	1:89:A:ILE:HD12	6	0.14
(3,28)	1:85:A:LEU:HD13	1:89:A:ILE:HD13	6	0.14
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD11	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD12	9	0.14
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD13	9	0.14
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD11	9	0.14
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD12	9	0.14
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD13	9	0.14
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD11	9	0.14
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD12	9	0.14
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD13	9	0.14
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD11	9	0.14
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD12	9	0.14
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD13	9	0.14
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD11	9	0.14
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD12	9	0.14
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD13	9	0.14
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD11	9	0.14
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD12	9	0.14
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD13	9	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG11	7	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG12	7	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG13	7	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG21	7	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG22	7	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG23	7	0.14
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG11	7	0.14
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG12	7	0.14
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG13	7	0.14
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG21	7	0.14
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG22	7	0.14
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG23	7	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG11	7	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG12	7	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG13	7	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG21	7	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG22	7	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG23	7	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG11	8	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG12	8	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG13	8	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG21	8	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG22	8	0.14
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG23	8	0.14
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG11	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG12	8	0.14
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG13	8	0.14
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG21	8	0.14
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG22	8	0.14
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG23	8	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG11	8	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG12	8	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG13	8	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG21	8	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG22	8	0.14
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG23	8	0.14
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD11	7	0.14
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD12	7	0.14
(2,474)	2:95:B:CYS:SG	1:89:A:ILE:HD13	7	0.14
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD11	8	0.14
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD12	8	0.14
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD13	8	0.14
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD21	8	0.14
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD22	8	0.14
(2,452)	2:41:B:CYS:SG	1:74:A:LEU:HD23	8	0.14
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD11	8	0.14
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD12	8	0.14
(2,403)	1:39:A:CYS:SG	2:101:B:ILE:HD13	8	0.14
(2,158)	2:30:B:LEU:CG	1:45:A:TRP:H	9	0.14
(2,102)	1:41:A:CYS:SG	2:57:B:GLY:H	7	0.14
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD11	8	0.13
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD12	8	0.13
(3,20)	1:7:A:LEU:HD11	1:62:A:ILE:HD13	8	0.13
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD11	8	0.13
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD12	8	0.13
(3,20)	1:7:A:LEU:HD12	1:62:A:ILE:HD13	8	0.13
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD11	8	0.13
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD12	8	0.13
(3,20)	1:7:A:LEU:HD13	1:62:A:ILE:HD13	8	0.13
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD11	8	0.13
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD12	8	0.13
(3,20)	1:7:A:LEU:HD21	1:62:A:ILE:HD13	8	0.13
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD11	8	0.13
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD12	8	0.13
(3,20)	1:7:A:LEU:HD22	1:62:A:ILE:HD13	8	0.13
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD11	8	0.13
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD12	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,20)	1:7:A:LEU:HD23	1:62:A:ILE:HD13	8	0.13
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG11	5	0.13
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG12	5	0.13
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG13	5	0.13
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG21	5	0.13
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG22	5	0.13
(3,9)	2:62:B:ILE:HD11	2:98:B:VAL:HG23	5	0.13
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG11	5	0.13
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG12	5	0.13
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG13	5	0.13
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG21	5	0.13
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG22	5	0.13
(3,9)	2:62:B:ILE:HD12	2:98:B:VAL:HG23	5	0.13
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG11	5	0.13
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG12	5	0.13
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG13	5	0.13
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG21	5	0.13
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG22	5	0.13
(3,9)	2:62:B:ILE:HD13	2:98:B:VAL:HG23	5	0.13
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD11	9	0.13
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD12	9	0.13
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD13	9	0.13
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD21	9	0.13
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD22	9	0.13
(2,472)	2:95:B:CYS:SG	1:85:A:LEU:HD23	9	0.13
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD11	8	0.13
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD12	8	0.13
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD13	8	0.13
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD21	8	0.13
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD22	8	0.13
(1,449)	1:39:A:CYS:SG	1:73:A:LEU:HD23	8	0.13
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD11	6	0.13
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD12	6	0.13
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD13	6	0.13
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD21	6	0.13
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD22	6	0.13
(1,429)	1:5:A:ILE:CG1	1:83:A:LEU:HD23	6	0.13
(1,303)	2:39:B:CYS:SG	2:31:B:TRP:H	5	0.13
(1,284)	2:5:B:ILE:CG1	2:106:B:ARG:H	7	0.13
(6,155)	2:43:B:SER:O	2:47:B:LEU:H	8	0.12
(6,153)	2:42:B:ALA:O	2:46:B:LEU:H	1	0.12
(6,101)	1:95:A:CYS:O	1:99:A:LEU:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,28)	1:37:A:ILE:N	1:33:A:SER:O	9	0.12
(5,16)	2:26:B:GLY:CA	2:25:B:GLU:CD	2	0.12
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD11	5	0.12
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD12	5	0.12
(3,21)	1:34:A:VAL:HG11	1:38:A:ILE:HD13	5	0.12
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD11	5	0.12
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD12	5	0.12
(3,21)	1:34:A:VAL:HG12	1:38:A:ILE:HD13	5	0.12
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD11	5	0.12
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD12	5	0.12
(3,21)	1:34:A:VAL:HG13	1:38:A:ILE:HD13	5	0.12
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD11	5	0.12
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD12	5	0.12
(3,21)	1:34:A:VAL:HG21	1:38:A:ILE:HD13	5	0.12
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD11	5	0.12
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD12	5	0.12
(3,21)	1:34:A:VAL:HG22	1:38:A:ILE:HD13	5	0.12
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD11	5	0.12
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD12	5	0.12
(3,21)	1:34:A:VAL:HG23	1:38:A:ILE:HD13	5	0.12
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD11	6	0.12
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD12	6	0.12
(1,498)	1:95:A:CYS:SG	1:89:A:ILE:HD13	6	0.12
(1,220)	1:95:A:CYS:SG	1:90:A:GLY:H	10	0.12
(1,219)	1:95:A:CYS:SG	1:89:A:ILE:H	3	0.12
(6,102)	1:99:A:LEU:N	1:95:A:CYS:O	7	0.11
(6,28)	1:37:A:ILE:N	1:33:A:SER:O	8	0.11
(3,38)	2:63:B:TRP:CD1	2:47:B:LEU:CD1	10	0.11
(3,38)	2:63:B:TRP:CD1	2:47:B:LEU:CD2	10	0.11
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD11	2	0.11
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD12	2	0.11
(2,393)	1:39:A:CYS:SG	2:54:B:ILE:HD13	2	0.11
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD11	6	0.11
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD12	6	0.11
(2,390)	1:39:A:CYS:SG	2:11:B:ILE:HD13	6	0.11
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD11	8	0.11
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD12	8	0.11
(1,519)	2:39:B:CYS:SG	2:5:B:ILE:HD13	8	0.11
(1,284)	2:5:B:ILE:CG1	2:106:B:ARG:H	6	0.11
(1,177)	1:95:A:CYS:SG	1:7:A:LEU:H	5	0.11
(1,72)	1:39:A:CYS:SG	1:25:A:GLU:H	7	0.11
(6,158)	2:48:B:ALA:N	2:44:B:PHE:O	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,39)	2:63:B:TRP:CD1	2:62:B:ILE:CG2	10	0.1
(2,421)	1:41:A:CYS:SG	2:101:B:ILE:HD11	4	0.1
(2,421)	1:41:A:CYS:SG	2:101:B:ILE:HD12	4	0.1
(2,421)	1:41:A:CYS:SG	2:101:B:ILE:HD13	4	0.1
(1,214)	1:95:A:CYS:SG	1:81:A:GLN:H	4	0.1

10 Dihedral-angle violation analysis ⓘ

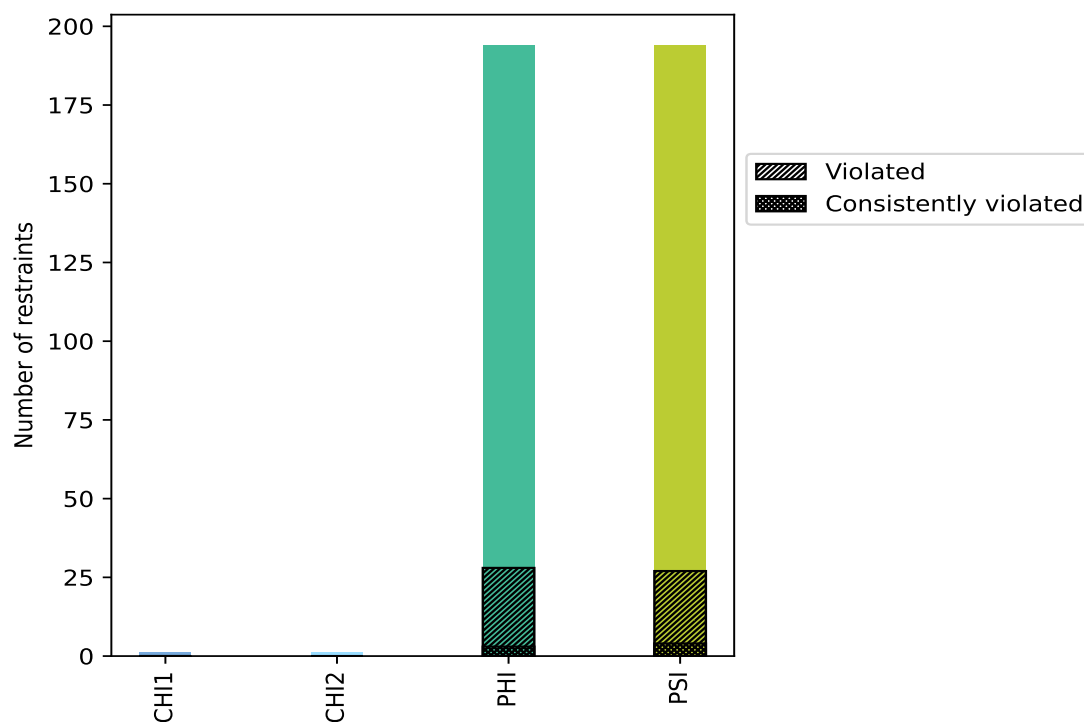
10.1 Summary of dihedral-angle violations ⓘ

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	1	0.3	0	0.0	0.0	0	0.0	0.0
CHI2	1	0.3	0	0.0	0.0	0	0.0	0.0
PHI	194	49.7	28	14.4	7.2	3	1.5	0.8
PSI	194	49.7	27	13.9	6.9	4	2.1	1.0
Total	390	100.0	55	14.1	14.1	7	1.8	1.8

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 ⓘ



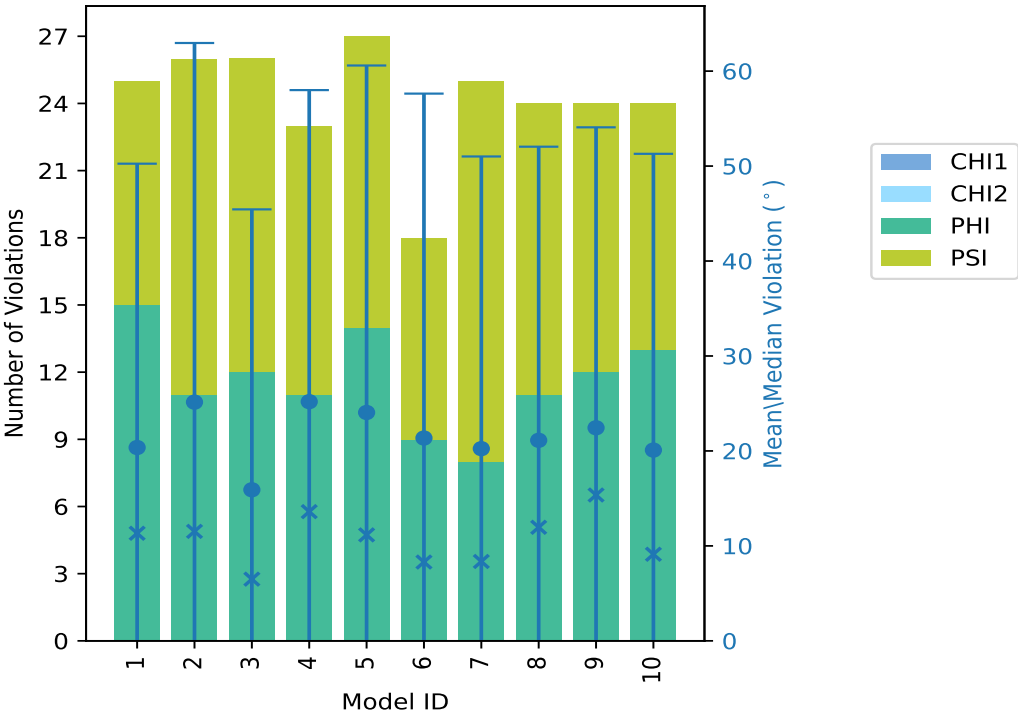
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

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	CHI2	PHI	PSI	Total				
1	0	0	15	10	25	20.36	158.29	29.89	11.33
2	0	0	11	15	26	25.14	157.15	37.82	11.53
3	0	0	12	14	26	15.91	155.1	29.53	6.5
4	0	0	11	12	23	25.19	156.3	32.81	13.61
5	0	0	14	13	27	24.05	155.99	36.54	11.16
6	0	0	9	9	18	21.36	157.48	36.27	8.3
7	0	0	8	17	25	20.24	158.57	30.77	8.36
8	0	0	11	13	24	21.12	157.3	30.92	11.96
9	0	0	12	12	24	22.44	158.86	31.64	15.36
10	0	0	13	11	24	20.09	157.45	31.2	9.12

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

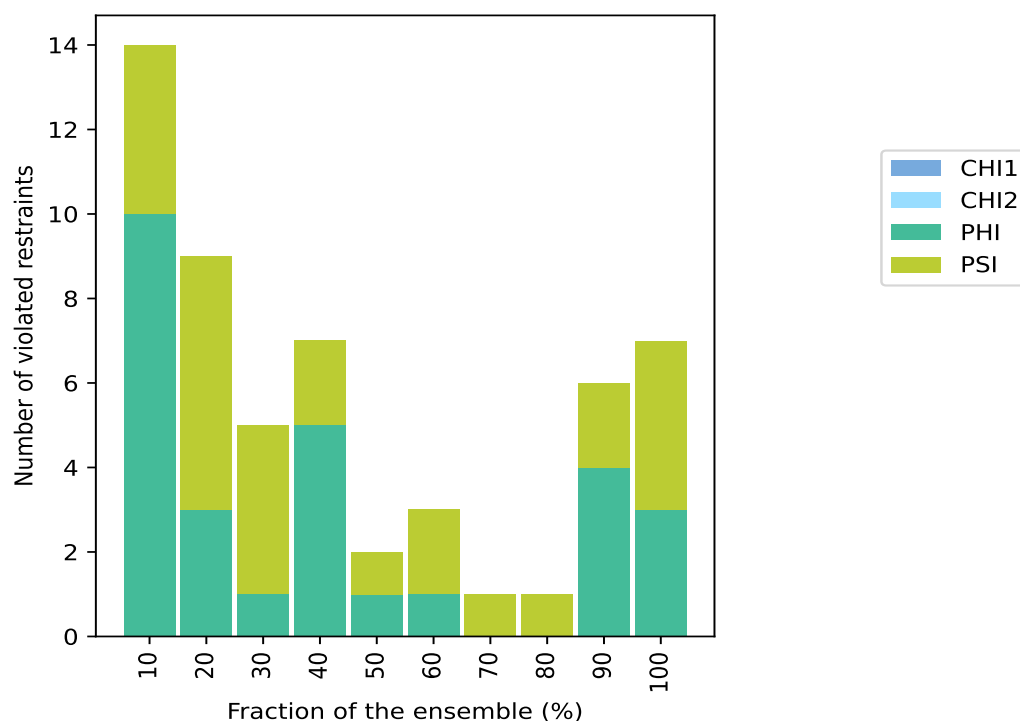
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	CHI2	PHI	PSI	Total	Count ¹	%
0	0	10	4	14	1	10.0
0	0	3	6	9	2	20.0
0	0	1	4	5	3	30.0
0	0	5	2	7	4	40.0
0	0	1	1	2	5	50.0
0	0	1	2	3	6	60.0
0	0	0	1	1	7	70.0
0	0	0	1	1	8	80.0
0	0	4	2	6	9	90.0
0	0	3	4	7	10	100.0

¹ Number of models with violations

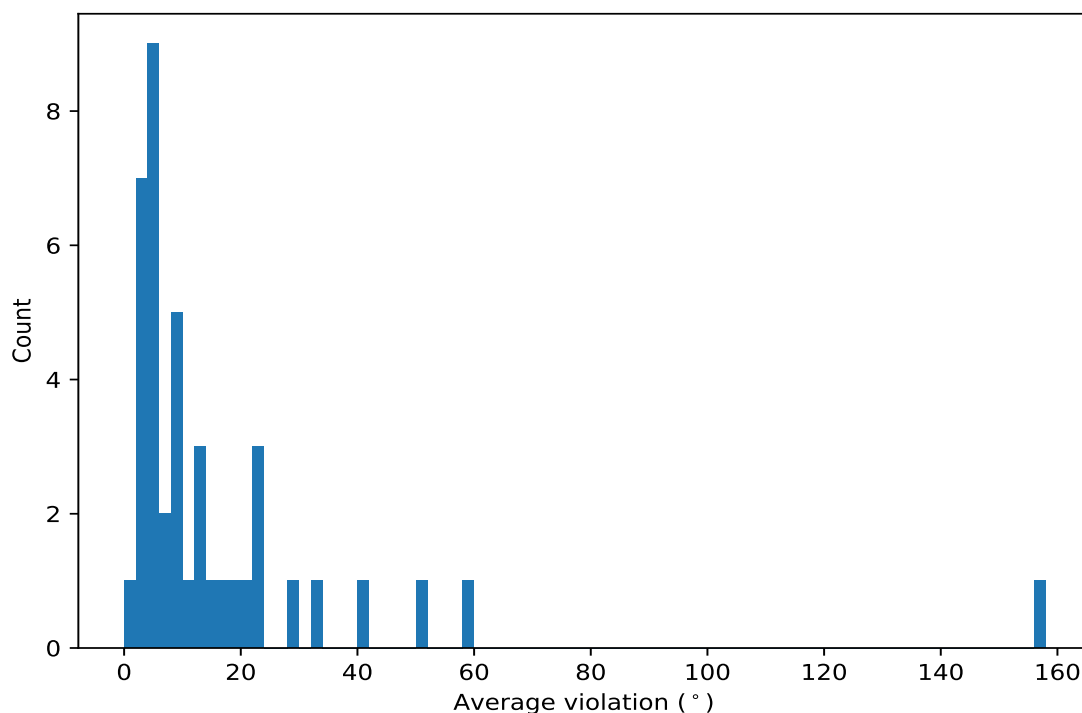
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	10	157.25	1.12	157.38
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	10	29.41	2.47	28.58
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	10	22.91	9.6	25.58
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	10	20.38	5.03	20.98
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	10	16.44	1.15	16.62
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	10	8.19	1.82	8.53
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	10	6.27	1.21	6.3
(1,339)	2:81:B:GLN:C	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	9	40.65	8.95	43.01
(1,3)	1:1:A:MET:C	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	9	32.74	18.57	23.63
(1,141)	1:77:A:GLY:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	9	13.91	6.59	11.16
(1,336)	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	2:79:B:PHE:N	9	10.05	4.3	11.63
(1,335)	2:77:B:GLY:C	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	9	9.76	1.98	8.89
(1,188)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:LEU:N	9	5.25	1.74	4.75

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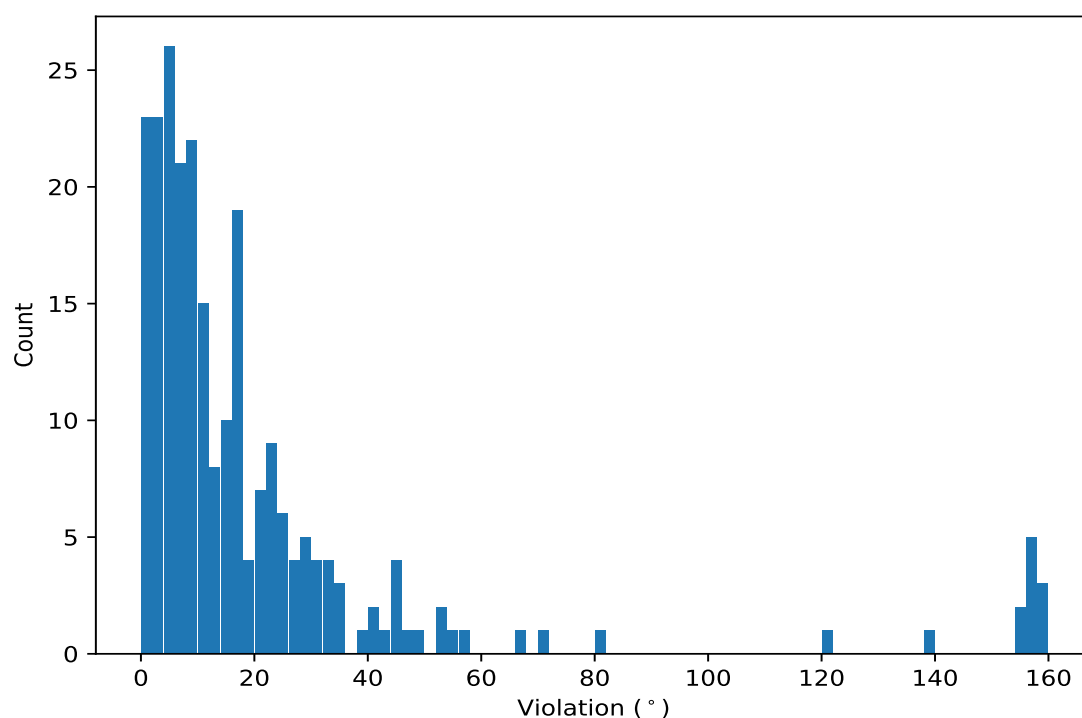
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,382)	2:103:B:LEU:N	2:103:B:LEU:CA	2:103:B:LEU:C	2:104:B:LEU:N	8	1.79	0.81	1.44
(1,338)	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	2:80:B:GLY:N	7	58.51	48.78	28.92
(1,342)	2:83:B:LEU:N	2:83:B:LEU:CA	2:83:B:LEU:C	2:84:B:ASP:N	6	51.24	14.9	49.3
(1,290)	2:55:B:PRO:N	2:55:B:PRO:CA	2:55:B:PRO:C	2:56:B:THR:N	6	14.12	8.64	15.02
(1,99)	1:54:A:ILE:C	1:55:A:PRO:N	1:55:A:PRO:CA	1:55:A:PRO:C	6	2.56	1.57	1.91
(1,96)	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	1:54:A:ILE:N	5	23.62	14.57	19.01
(1,97)	1:53:A:TYR:C	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	5	3.85	3.51	1.91
(1,278)	2:49:B:GLN:N	2:49:B:GLN:CA	2:49:B:GLN:C	2:50:B:THR:N	4	19.46	2.64	19.23
(1,337)	2:78:B:PHE:C	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	4	13.17	4.83	15.54
(1,149)	1:81:A:GLN:C	1:82:A:ARG:N	1:82:A:ARG:CA	1:82:A:ARG:C	4	6.38	3.56	5.94
(1,277)	2:48:B:ALA:C	2:49:B:GLN:N	2:49:B:GLN:CA	2:49:B:GLN:C	4	5.83	0.97	5.88
(1,283)	2:51:B:LEU:C	2:52:B:ALA:N	2:52:B:ALA:CA	2:52:B:ALA:C	4	4.59	3.44	4.22
(1,284)	2:52:B:ALA:N	2:52:B:ALA:CA	2:52:B:ALA:C	2:53:B:TYR:N	4	3.62	2.01	2.86
(1,151)	1:82:A:ARG:C	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	4	2.12	0.93	1.92
(1,92)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:ALA:N	3	22.03	3.1	23.16
(1,121)	1:65:A:GLY:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	3	12.42	3.17	14.19
(1,344)	2:84:B:ASP:N	2:84:B:ASP:CA	2:84:B:ASP:C	2:85:B:LEU:N	3	4.89	2.78	3.71
(1,50)	1:30:A:LEU:N	1:30:A:LEU:CA	1:30:A:LEU:C	1:31:A:TRP:N	3	4.47	1.47	3.57
(1,340)	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	2:83:B:LEU:N	3	4.14	1.54	5.09
(1,240)	2:30:B:LEU:N	2:30:B:LEU:CA	2:30:B:LEU:C	2:31:B:TRP:N	2	9.71	1.92	9.71
(1,93)	1:51:A:LEU:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	2	8.72	2.6	8.72
(1,95)	1:52:A:ALA:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	2	8.35	2.53	8.35
(1,332)	2:76:B:TRP:N	2:76:B:TRP:CA	2:76:B:TRP:C	2:77:B:GLY:N	2	5.72	3.19	5.72
(1,4)	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	1:3:A:PRO:N	2	4.85	0.35	4.85
(1,148)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:ARG:N	2	4.2	0.26	4.2
(1,389)	2:108:B:THR:C	2:109:B:PRO:N	2:109:B:PRO:CA	2:109:B:PRO:C	2	2.92	1.06	2.92
(1,150)	1:82:A:ARG:N	1:82:A:ARG:CA	1:82:A:ARG:C	1:83:A:LEU:N	2	2.55	0.53	2.55
(1,94)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:TYR:N	2	2.05	0.86	2.05

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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 (°)
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	9	158.86
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	7	158.57
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	1	158.29
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	6	157.48
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	10	157.45
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	8	157.3
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	2	157.15
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	4	156.3
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	5	155.99
(1,386)	2:105:B:SER:N	2:105:B:SER:CA	2:105:B:SER:C	2:106:B:ARG:N	3	155.1
(1,338)	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	2:80:B:GLY:N	2	138.91
(1,338)	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	2:80:B:GLY:N	5	120.55
(1,342)	2:83:B:LEU:N	2:83:B:LEU:CA	2:83:B:LEU:C	2:84:B:ASP:N	5	80.3
(1,338)	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	2:80:B:GLY:N	4	71.69
(1,3)	1:1:A:MET:C	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	6	66.5
(1,3)	1:1:A:MET:C	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	9	57.05
(1,342)	2:83:B:LEU:N	2:83:B:LEU:CA	2:83:B:LEU:C	2:84:B:ASP:N	2	55.7
(1,339)	2:81:B:GLN:C	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	7	53.92
(1,342)	2:83:B:LEU:N	2:83:B:LEU:CA	2:83:B:LEU:C	2:84:B:ASP:N	4	52.05
(1,96)	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	1:54:A:ILE:N	8	48.26
(1,342)	2:83:B:LEU:N	2:83:B:LEU:CA	2:83:B:LEU:C	2:84:B:ASP:N	1	46.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,339)	2:81:B:GLN:C	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	4	45.75
(1,3)	1:1:A:MET:C	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	5	45.03
(1,339)	2:81:B:GLN:C	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	2	44.61
(1,339)	2:81:B:GLN:C	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	8	44.38
(1,339)	2:81:B:GLN:C	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	3	43.01
(1,339)	2:81:B:GLN:C	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	9	41.92
(1,339)	2:81:B:GLN:C	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	10	40.63
(1,342)	2:83:B:LEU:N	2:83:B:LEU:CA	2:83:B:LEU:C	2:84:B:ASP:N	10	38.0
(1,3)	1:1:A:MET:C	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	10	35.43
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	10	34.85
(1,342)	2:83:B:LEU:N	2:83:B:LEU:CA	2:83:B:LEU:C	2:84:B:ASP:N	9	34.8
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	4	33.85
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	9	33.17
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	8	32.99
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	3	32.38
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	5	31.77
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	9	31.64
(1,96)	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	1:54:A:ILE:N	7	31.03
(1,339)	2:81:B:GLN:C	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	5	30.4
(1,338)	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	2:80:B:GLY:N	7	28.92
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	6	28.58
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	7	28.57
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	8	28.45
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	1	28.44
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	7	27.71
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	2	27.22
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	4	27.17
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	4	26.7
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	1	25.91
(1,141)	1:77:A:GLY:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	1	25.64
(1,287)	2:53:B:TYR:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	10	25.32
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	7	25.31
(1,92)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:ALA:N	1	25.14
(1,187)	1:102:A:ASN:C	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	2	24.18
(1,3)	1:1:A:MET:C	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	4	23.63
(1,290)	2:55:B:PRO:N	2:55:B:PRO:CA	2:55:B:PRO:C	2:56:B:THR:N	6	23.5
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	1	23.44
(1,92)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:ALA:N	7	23.16
(1,186)	1:102:A:ASN:N	1:102:A:ASN:CA	1:102:A:ASN:C	1:103:A:LEU:N	2	23.12
(1,278)	2:49:B:GLN:N	2:49:B:GLN:CA	2:49:B:GLN:C	2:50:B:THR:N	10	23.11
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	8	23.02
(1,290)	2:55:B:PRO:N	2:55:B:PRO:CA	2:55:B:PRO:C	2:56:B:THR:N	3	22.23
(1,3)	1:1:A:MET:C	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	2	22.08
(1,141)	1:77:A:GLY:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	2	21.98
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	10	21.96
(1,290)	2:55:B:PRO:N	2:55:B:PRO:CA	2:55:B:PRO:C	2:56:B:THR:N	5	21.68
(1,3)	1:1:A:MET:C	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	3	21.57
(1,339)	2:81:B:GLN:C	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	1	21.23
(1,278)	2:49:B:GLN:N	2:49:B:GLN:CA	2:49:B:GLN:C	2:50:B:THR:N	4	20.72
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	9	20.01
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	2	19.87

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	1:54:A:ILE:N	9	19.01
(1,341)	2:82:B:ARG:C	2:83:B:LEU:N	2:83:B:LEU:CA	2:83:B:LEU:C	5	18.34
(1,141)	1:77:A:GLY:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	8	18.09
(1,338)	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	2:80:B:GLY:N	8	17.9
(1,92)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:ALA:N	9	17.8
(1,278)	2:49:B:GLN:N	2:49:B:GLN:CA	2:49:B:GLN:C	2:50:B:THR:N	9	17.73
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	8	17.71
(1,5)	1:2:A:ASN:C	1:3:A:PRO:N	1:3:A:PRO:CA	1:3:A:PRO:C	6	17.7
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2	17.43
(1,191)	1:104:A:LEU:C	1:105:A:SER:N	1:105:A:SER:CA	1:105:A:SER:C	5	17.41
(1,141)	1:77:A:GLY:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	4	17.13
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	10	17.12
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	7	16.81
(1,337)	2:78:B:PHE:C	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	8	16.66
(1,337)	2:78:B:PHE:C	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	1	16.65
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	6	16.64
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	9	16.61
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	1	16.44
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	4	16.43
(1,278)	2:49:B:GLN:N	2:49:B:GLN:CA	2:49:B:GLN:C	2:50:B:THR:N	7	16.3
(1,338)	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	2:80:B:GLY:N	9	16.29
(1,190)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:SER:N	2	16.27
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	5	15.82
(1,338)	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	2:80:B:GLY:N	1	15.34
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	6	15.23
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	3	15.14
(1,121)	1:65:A:GLY:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	5	15.09
(1,336)	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	2:79:B:PHE:N	8	14.86
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	6	14.46
(1,337)	2:78:B:PHE:C	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	9	14.43
(1,387)	2:107:B:SER:C	2:108:B:THR:N	2:108:B:THR:CA	2:108:B:THR:C	3	14.19
(1,121)	1:65:A:GLY:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	10	14.19
(1,336)	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	2:79:B:PHE:N	4	13.61
(1,335)	2:77:B:GLY:C	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	3	13.53
(1,383)	2:103:B:LEU:C	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	3	13.34
(1,3)	1:1:A:MET:C	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	8	13.2
(1,336)	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	2:79:B:PHE:N	7	12.99
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	3	12.71
(1,336)	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	2:79:B:PHE:N	1	12.68
(1,335)	2:77:B:GLY:C	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	10	12.43
(1,336)	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	2:79:B:PHE:N	9	11.63
(1,240)	2:30:B:LEU:N	2:30:B:LEU:CA	2:30:B:LEU:C	2:31:B:TRP:N	5	11.63
(1,336)	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	2:79:B:PHE:N	5	11.57
(1,149)	1:81:A:GLN:C	1:82:A:ARG:N	1:82:A:ARG:CA	1:82:A:ARG:C	2	11.57
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	4	11.54
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2	11.49
(1,185)	1:101:A:ILE:C	1:102:A:ASN:N	1:102:A:ASN:CA	1:102:A:ASN:C	2	11.41
(1,93)	1:51:A:LEU:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1	11.33
(1,141)	1:77:A:GLY:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	5	11.16
(1,335)	2:77:B:GLY:C	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	4	10.97
(1,95)	1:52:A:ALA:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	7	10.88

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	1:54:A:ILE:N	4	10.74
(1,97)	1:53:A:TYR:C	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	8	10.72
(1,280)	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	2:51:B:LEU:N	5	10.65
(1,3)	1:1:A:MET:C	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	1	10.16
(1,335)	2:77:B:GLY:C	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	2	9.64
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	1	9.29
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	10	9.17
(1,141)	1:77:A:GLY:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	6	9.09
(1,96)	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	1:54:A:ILE:N	10	9.06
(1,279)	2:49:B:GLN:C	2:50:B:THR:N	2:50:B:THR:CA	2:50:B:THR:C	5	8.94
(1,332)	2:76:B:TRP:N	2:76:B:TRP:CA	2:76:B:TRP:C	2:77:B:GLY:N	4	8.9
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	8	8.89
(1,335)	2:77:B:GLY:C	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	1	8.89
(1,188)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:LEU:N	2	8.78
(1,283)	2:51:B:LEU:C	2:52:B:ALA:N	2:52:B:ALA:CA	2:52:B:ALA:C	1	8.74
(1,344)	2:84:B:ASP:N	2:84:B:ASP:CA	2:84:B:ASP:C	2:85:B:LEU:N	4	8.72
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	9	8.57
(1,335)	2:77:B:GLY:C	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	5	8.57
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	2	8.49
(1,193)	2:1:B:MET:C	2:2:B:ASN:N	2:2:B:ASN:CA	2:2:B:ASN:C	1	8.49
(1,335)	2:77:B:GLY:C	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	7	8.36
(1,290)	2:55:B:PRO:N	2:55:B:PRO:CA	2:55:B:PRO:C	2:56:B:THR:N	7	8.35
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	7	8.33
(1,141)	1:77:A:GLY:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	3	8.27
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	4	8.03
(1,335)	2:77:B:GLY:C	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	8	8.02
(1,121)	1:65:A:GLY:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	3	7.97
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	8	7.83
(1,240)	2:30:B:LEU:N	2:30:B:LEU:CA	2:30:B:LEU:C	2:31:B:TRP:N	8	7.79
(1,188)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:LEU:N	1	7.74
(1,149)	1:81:A:GLN:C	1:82:A:ARG:N	1:82:A:ARG:CA	1:82:A:ARG:C	6	7.52
(1,335)	2:77:B:GLY:C	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	9	7.42
(1,290)	2:55:B:PRO:N	2:55:B:PRO:CA	2:55:B:PRO:C	2:56:B:THR:N	1	7.42
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	2	7.26
(1,283)	2:51:B:LEU:C	2:52:B:ALA:N	2:52:B:ALA:CA	2:52:B:ALA:C	8	7.23
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	6	7.14
(1,141)	1:77:A:GLY:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	9	7.11
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	7	7.05
(1,284)	2:52:B:ALA:N	2:52:B:ALA:CA	2:52:B:ALA:C	2:53:B:TYR:N	8	6.95
(1,277)	2:48:B:ALA:C	2:49:B:GLN:N	2:49:B:GLN:CA	2:49:B:GLN:C	7	6.88
(1,141)	1:77:A:GLY:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	10	6.72
(1,277)	2:48:B:ALA:C	2:49:B:GLN:N	2:49:B:GLN:CA	2:49:B:GLN:C	10	6.71
(1,50)	1:30:A:LEU:N	1:30:A:LEU:CA	1:30:A:LEU:C	1:31:A:TRP:N	3	6.54
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	1	6.52
(1,336)	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	2:79:B:PHE:N	3	6.46
(1,93)	1:51:A:LEU:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	7	6.12
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	5	6.08
(1,99)	1:54:A:ILE:C	1:55:A:PRO:N	1:55:A:PRO:CA	1:55:A:PRO:C	10	5.98
(1,333)	2:76:B:TRP:C	2:77:B:GLY:N	2:77:B:GLY:CA	2:77:B:GLY:C	4	5.92
(1,95)	1:52:A:ALA:C	1:53:A:TYR:N	1:53:A:TYR:CA	1:53:A:TYR:C	1	5.82
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	3	5.58

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	10	5.5
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	9	5.45
(1,340)	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	2:83:B:LEU:N	7	5.36
(1,188)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:LEU:N	3	5.29
(1,188)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:LEU:N	6	5.25
(1,4)	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	1:3:A:PRO:N	8	5.2
(1,336)	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	2:79:B:PHE:N	2	5.16
(1,192)	1:105:A:SER:N	1:105:A:SER:CA	1:105:A:SER:C	1:106:A:ARG:N	7	5.13
(1,340)	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	2:83:B:LEU:N	3	5.09
(1,277)	2:48:B:ALA:C	2:49:B:GLN:N	2:49:B:GLN:CA	2:49:B:GLN:C	9	5.06
(1,337)	2:78:B:PHE:C	2:79:B:PHE:N	2:79:B:PHE:CA	2:79:B:PHE:C	5	4.95
(1,152)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ASP:N	7	4.92
(1,384)	2:104:B:LEU:N	2:104:B:LEU:CA	2:104:B:LEU:C	2:105:B:SER:N	5	4.88
(1,188)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:LEU:N	10	4.75
(1,277)	2:48:B:ALA:C	2:49:B:GLN:N	2:49:B:GLN:CA	2:49:B:GLN:C	4	4.68
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	3	4.5
(1,236)	2:23:B:PHE:N	2:23:B:PHE:CA	2:23:B:PHE:C	2:24:B:SER:N	6	4.5
(1,4)	1:2:A:ASN:N	1:2:A:ASN:CA	1:2:A:ASN:C	1:3:A:PRO:N	3	4.5
(1,148)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:ARG:N	7	4.47
(1,149)	1:81:A:GLN:C	1:82:A:ARG:N	1:82:A:ARG:CA	1:82:A:ARG:C	9	4.36
(1,188)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:LEU:N	9	4.34
(1,188)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:LEU:N	8	4.15
(1,389)	2:108:B:THR:C	2:109:B:PRO:N	2:109:B:PRO:CA	2:109:B:PRO:C	10	3.99
(1,148)	1:81:A:GLN:N	1:81:A:GLN:CA	1:81:A:GLN:C	1:82:A:ARG:N	3	3.94
(1,344)	2:84:B:ASP:N	2:84:B:ASP:CA	2:84:B:ASP:C	2:85:B:LEU:N	6	3.71
(1,173)	1:95:A:CYS:C	1:96:A:ALA:N	1:96:A:ALA:CA	1:96:A:ALA:C	1	3.68
(1,188)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:LEU:N	5	3.6
(1,151)	1:82:A:ARG:C	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	5	3.58
(1,50)	1:30:A:LEU:N	1:30:A:LEU:CA	1:30:A:LEU:C	1:31:A:TRP:N	8	3.57
(1,97)	1:53:A:TYR:C	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1	3.47
(1,284)	2:52:B:ALA:N	2:52:B:ALA:CA	2:52:B:ALA:C	2:53:B:TYR:N	3	3.4
(1,188)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:LEU:N	7	3.33
(1,50)	1:30:A:LEU:N	1:30:A:LEU:CA	1:30:A:LEU:C	1:31:A:TRP:N	10	3.3
(1,382)	2:103:B:LEU:N	2:103:B:LEU:CA	2:103:B:LEU:C	2:104:B:LEU:N	5	3.21
(1,150)	1:82:A:ARG:N	1:82:A:ARG:CA	1:82:A:ARG:C	1:83:A:LEU:N	2	3.08
(1,382)	2:103:B:LEU:N	2:103:B:LEU:CA	2:103:B:LEU:C	2:104:B:LEU:N	3	2.91
(1,94)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:TYR:N	5	2.91
(1,332)	2:76:B:TRP:N	2:76:B:TRP:CA	2:76:B:TRP:C	2:77:B:GLY:N	7	2.53
(1,99)	1:54:A:ILE:C	1:55:A:PRO:N	1:55:A:PRO:CA	1:55:A:PRO:C	4	2.52
(1,284)	2:52:B:ALA:N	2:52:B:ALA:CA	2:52:B:ALA:C	2:53:B:TYR:N	6	2.33
(1,344)	2:84:B:ASP:N	2:84:B:ASP:CA	2:84:B:ASP:C	2:85:B:LEU:N	2	2.23
(1,151)	1:82:A:ARG:C	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	10	2.12
(1,149)	1:81:A:GLN:C	1:82:A:ARG:N	1:82:A:ARG:CA	1:82:A:ARG:C	8	2.09
(1,382)	2:103:B:LEU:N	2:103:B:LEU:CA	2:103:B:LEU:C	2:104:B:LEU:N	9	2.08
(1,150)	1:82:A:ARG:N	1:82:A:ARG:CA	1:82:A:ARG:C	1:83:A:LEU:N	3	2.03
(1,99)	1:54:A:ILE:C	1:55:A:PRO:N	1:55:A:PRO:CA	1:55:A:PRO:C	6	1.97
(1,340)	2:82:B:ARG:N	2:82:B:ARG:CA	2:82:B:ARG:C	2:83:B:LEU:N	5	1.96
(1,97)	1:53:A:TYR:C	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	5	1.91
(1,389)	2:108:B:THR:C	2:109:B:PRO:N	2:109:B:PRO:CA	2:109:B:PRO:C	9	1.86
(1,99)	1:54:A:ILE:C	1:55:A:PRO:N	1:55:A:PRO:CA	1:55:A:PRO:C	2	1.85
(1,97)	1:53:A:TYR:C	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	6	1.85

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,284)	2:52:B:ALA:N	2:52:B:ALA:CA	2:52:B:ALA:C	2:53:B:TYR:N	2	1.8
(1,151)	1:82:A:ARG:C	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1	1.71
(1,382)	2:103:B:LEU:N	2:103:B:LEU:CA	2:103:B:LEU:C	2:104:B:LEU:N	10	1.64
(1,99)	1:54:A:ILE:C	1:55:A:PRO:N	1:55:A:PRO:CA	1:55:A:PRO:C	3	1.56
(1,290)	2:55:B:PRO:N	2:55:B:PRO:CA	2:55:B:PRO:C	2:56:B:THR:N	8	1.53
(1,336)	2:78:B:PHE:N	2:78:B:PHE:CA	2:78:B:PHE:C	2:79:B:PHE:N	10	1.46
(1,99)	1:54:A:ILE:C	1:55:A:PRO:N	1:55:A:PRO:CA	1:55:A:PRO:C	9	1.45
(1,343)	2:83:B:LEU:C	2:84:B:ASP:N	2:84:B:ASP:CA	2:84:B:ASP:C	5	1.37
(1,97)	1:53:A:TYR:C	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	3	1.29
(1,382)	2:103:B:LEU:N	2:103:B:LEU:CA	2:103:B:LEU:C	2:104:B:LEU:N	4	1.23
(1,382)	2:103:B:LEU:N	2:103:B:LEU:CA	2:103:B:LEU:C	2:104:B:LEU:N	2	1.22
(1,283)	2:51:B:LEU:C	2:52:B:ALA:N	2:52:B:ALA:CA	2:52:B:ALA:C	10	1.2
(1,94)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:TYR:N	2	1.19
(1,283)	2:51:B:LEU:C	2:52:B:ALA:N	2:52:B:ALA:CA	2:52:B:ALA:C	3	1.18
(1,151)	1:82:A:ARG:C	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	4	1.06
(1,382)	2:103:B:LEU:N	2:103:B:LEU:CA	2:103:B:LEU:C	2:104:B:LEU:N	6	1.01
(1,382)	2:103:B:LEU:N	2:103:B:LEU:CA	2:103:B:LEU:C	2:104:B:LEU:N	7	1.01