



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 6FVC / pdb_00006fvc
BMRB ID : 34240
Title : Protein environment affects the water-tryptophan binding mode. Molecular dynamics simulations of Engrailed homeodomain mutants
Authors : Trosanova, Z.; Zachrdla, M.; Jansen, S.; Srb, P.; Zidek, L.; Kozelka, J.
Deposited on : 2018-03-02

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

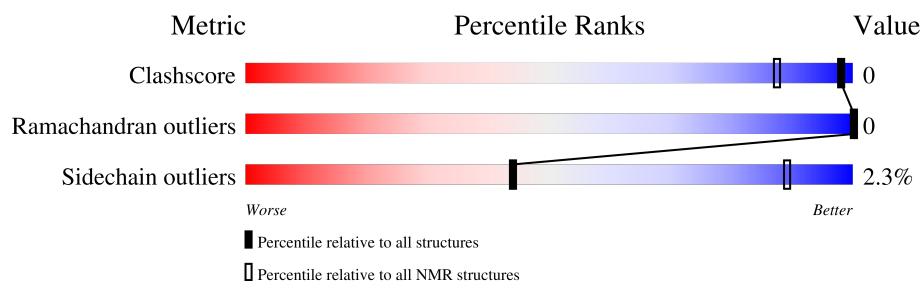
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	64	31% 39% . 28%

2 Ensemble composition and analysis

This entry contains 3 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:11-A:56 (46)	0.35	3

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1087 atoms, of which 550 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Segmentation polarity homeobox protein engrailed.

Mol	Chain	Residues	Atoms						Trace
1	A	64	Total	C	H	N	O	S	0
			1084	329	548	107	99	1	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P02836
A	2	ALA	-	expression tag	UNP P02836
A	3	MET	-	expression tag	UNP P02836
A	55	GLU	LYS	engineered mutation	UNP P02836
A	63	GLY	-	expression tag	UNP P02836
A	64	SER	-	expression tag	UNP P02836

- Molecule 2 is water.

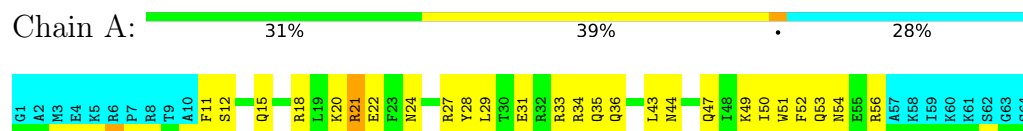
Mol	Chain	Residues	Atoms		
2	A	1	Total	H	O
			3	2	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Segmentation polarity homeobox protein engrailed

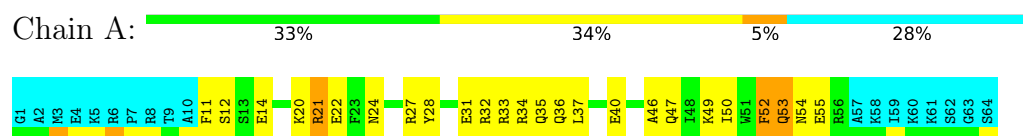


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

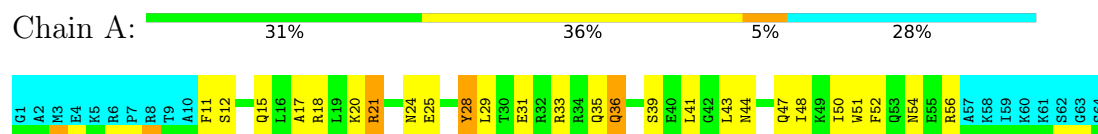
4.2.1 Score per residue for model 1

- Molecule 1: Segmentation polarity homeobox protein engrailed



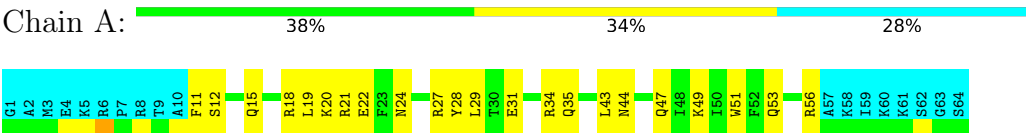
4.2.2 Score per residue for model 2

- Molecule 1: Segmentation polarity homeobox protein engrailed



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Segmentation polarity homeobox protein engrailed



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 3 were deposited, based on the following criterion: *three representative structures for the conformational equilibrium along the torsion angle N-CA-CB-CG of asparagine N51*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	

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	466
Number of shifts mapped to atoms	466
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.13±0.03	12±2/409 (2.9± 0.5%)	2.53±0.07	28±2/546 (5.1± 0.4%)
All	All	2.13	35/1227 (2.9%)	2.53	83/1638 (5.1%)

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	1.7±1.2
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	11	PHE	CA-C	8.01	1.62	1.52	3	1
1	A	31	GLU	N-CA	7.88	1.55	1.46	1	1
1	A	44	ASN	CA-CB	7.84	1.65	1.53	2	1
1	A	18	ARG	CZ-NH1	-7.69	1.22	1.32	2	1
1	A	21	ARG	CA-C	7.40	1.62	1.52	1	1
1	A	31	GLU	CA-C	7.33	1.62	1.52	2	1
1	A	36	GLN	N-CA	7.19	1.55	1.46	1	1
1	A	49	LYS	N-CA	7.16	1.55	1.46	3	1
1	A	14	GLU	CA-CB	6.95	1.64	1.53	1	1
1	A	12	SER	C-O	6.80	1.32	1.23	1	1
1	A	39	SER	N-CA	6.68	1.54	1.46	2	1
1	A	12	SER	CA-C	6.50	1.60	1.52	2	2
1	A	56	ARG	N-CA	6.36	1.54	1.46	3	1
1	A	34	ARG	CZ-NH1	-6.26	1.24	1.32	3	1
1	A	11	PHE	N-CA	5.97	1.53	1.45	2	1
1	A	36	GLN	CA-C	-5.91	1.45	1.52	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	43	LEU	N-CA	5.77	1.53	1.45	2	1
1	A	21	ARG	CA-CB	5.62	1.63	1.53	3	1
1	A	28	TYR	CA-C	5.62	1.59	1.52	3	1
1	A	25	GLU	N-CA	-5.62	1.39	1.46	2	1
1	A	18	ARG	N-CA	5.60	1.53	1.46	3	2
1	A	50	ILE	CA-CB	5.54	1.61	1.54	1	1
1	A	21	ARG	CZ-NH2	-5.43	1.26	1.33	1	1
1	A	28	TYR	N-CA	5.39	1.52	1.46	2	1
1	A	47	GLN	N-CA	5.37	1.53	1.46	2	1
1	A	29	LEU	N-CA	5.34	1.52	1.45	2	1
1	A	49	LYS	CA-C	5.29	1.59	1.52	1	1
1	A	40	GLU	CA-C	5.22	1.59	1.52	1	1
1	A	27	ARG	CZ-NH2	-5.10	1.26	1.33	1	1
1	A	55	GLU	N-CA	5.10	1.52	1.46	1	1
1	A	18	ARG	CA-CB	5.07	1.61	1.53	3	1
1	A	21	ARG	CZ-NH1	-5.06	1.25	1.32	3	1
1	A	12	SER	N-CA	5.02	1.51	1.45	1	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	PHE	CA-CB-CG	13.74	127.55	113.80	2	3
1	A	36	GLN	OE1-CD-NE2	-11.60	111.00	122.60	2	2
1	A	54	ASN	CA-CB-CG	10.99	123.59	112.60	2	2
1	A	52	PHE	CA-CB-CG	10.97	124.78	113.80	1	2
1	A	32	ARG	NE-CZ-NH1	10.70	132.20	121.50	1	1
1	A	32	ARG	NE-CZ-NH2	-10.42	109.82	119.20	1	1
1	A	35	GLN	OE1-CD-NE2	-10.15	112.45	122.60	1	1
1	A	47	GLN	OE1-CD-NE2	-8.20	114.40	122.60	3	2
1	A	17	ALA	CA-C-O	-8.15	111.83	120.63	2	1
1	A	15	GLN	OE1-CD-NE2	-7.79	114.81	122.60	3	1
1	A	53	GLN	OE1-CD-NE2	-7.71	114.89	122.60	3	2
1	A	24	ASN	CA-CB-CG	7.54	120.14	112.60	1	3
1	A	29	LEU	CA-C-N	7.40	136.29	123.05	3	1
1	A	29	LEU	C-N-CA	7.40	136.29	123.05	3	1
1	A	12	SER	CA-C-N	7.05	130.30	120.29	3	1
1	A	12	SER	C-N-CA	7.05	130.30	120.29	3	1
1	A	19	LEU	O-C-N	-6.98	114.83	122.09	3	1
1	A	49	LYS	N-CA-C	-6.81	103.78	111.07	1	1
1	A	36	GLN	CA-C-O	-6.63	113.86	120.82	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	48	ILE	CA-C-N	6.57	129.74	120.28	2	1
1	A	48	ILE	C-N-CA	6.57	129.74	120.28	2	1
1	A	43	LEU	O-C-N	-6.56	114.66	123.19	3	1
1	A	21	ARG	CD-NE-CZ	6.55	133.58	124.40	3	1
1	A	49	LYS	CA-C-N	6.33	131.59	121.34	3	1
1	A	49	LYS	C-N-CA	6.33	131.59	121.34	3	1
1	A	20	LYS	CA-C-N	6.29	133.13	122.26	3	3
1	A	20	LYS	C-N-CA	6.29	133.13	122.26	3	3
1	A	51	TRP	CA-C-N	6.23	129.48	120.38	3	2
1	A	51	TRP	C-N-CA	6.23	129.48	120.38	3	2
1	A	46	ALA	CA-C-N	6.17	128.55	120.28	1	1
1	A	46	ALA	C-N-CA	6.17	128.55	120.28	1	1
1	A	28	TYR	O-C-N	-6.13	116.43	122.99	2	1
1	A	36	GLN	CG-CD-NE2	6.13	125.59	116.40	2	1
1	A	19	LEU	CA-C-O	6.12	127.45	120.90	3	1
1	A	21	ARG	CA-C-O	6.07	126.83	119.31	1	1
1	A	33	ARG	CG-CD-NE	-5.98	98.84	112.00	1	1
1	A	44	ASN	CA-CB-CG	5.92	118.52	112.60	3	1
1	A	21	ARG	NE-CZ-NH1	5.85	127.35	121.50	2	1
1	A	51	TRP	CG-CD2-CE3	5.77	139.67	133.90	2	1
1	A	56	ARG	NH1-CZ-NH2	-5.71	111.88	119.30	3	1
1	A	33	ARG	CA-C-N	5.64	128.15	120.54	1	2
1	A	33	ARG	C-N-CA	5.64	128.15	120.54	1	2
1	A	21	ARG	NE-CZ-NH2	-5.60	114.16	119.20	2	1
1	A	27	ARG	NE-CZ-NH2	5.57	124.21	119.20	1	1
1	A	27	ARG	NH1-CZ-NH2	-5.56	112.08	119.30	1	1
1	A	35	GLN	CG-CD-NE2	5.55	124.72	116.40	1	1
1	A	31	GLU	CA-C-N	5.53	128.45	120.38	3	1
1	A	31	GLU	C-N-CA	5.53	128.45	120.38	3	1
1	A	27	ARG	NE-CZ-NH1	5.47	126.97	121.50	3	1
1	A	50	ILE	CB-CA-C	5.39	119.25	111.65	2	1
1	A	22	GLU	CA-C-N	5.38	127.48	120.28	3	1
1	A	22	GLU	C-N-CA	5.38	127.48	120.28	3	1
1	A	15	GLN	N-CA-CB	5.31	118.02	110.16	2	1
1	A	34	ARG	N-CA-CB	5.29	117.83	109.94	1	1
1	A	28	TYR	N-CA-CB	-5.25	102.93	111.22	1	1
1	A	24	ASN	OD1-CG-ND2	-5.21	117.39	122.60	1	1
1	A	51	TRP	CE2-CD2-CE3	-5.19	113.61	118.80	3	1
1	A	43	LEU	CA-C-N	5.14	129.93	121.39	2	1
1	A	43	LEU	C-N-CA	5.14	129.93	121.39	2	1
1	A	41	LEU	CA-C-O	-5.12	113.28	119.27	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	28	TYR	CA-C-N	5.06	130.41	122.21	2	1
1	A	28	TYR	C-N-CA	5.06	130.41	122.21	2	1
1	A	44	ASN	CB-CG-OD1	5.05	130.91	120.80	2	1
1	A	56	ARG	NE-CZ-NH1	5.05	126.55	121.50	2	1
1	A	49	LYS	CA-CB-CG	-5.04	104.01	114.10	3	1
1	A	18	ARG	NE-CZ-NH2	5.00	123.70	119.20	2	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	21	ARG	Sidechain	2
1	A	52	PHE	Sidechain	1
1	A	28	TYR	Sidechain	1
1	A	36	GLN	Mainchain	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	403	397	397	0±0
All	All	1212	1197	1191	1

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:GLU:HG3	1:A:37:LEU:HD21	0.41	1.93	1	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	46/64 (72%)	46±0 (99±1%)	0±0 (1±1%)	0±0 (0±0%)	100	100
All	All	138/192 (72%)	137 (99%)	1 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	43/56 (77%)	42±0 (98±0%)	1±0 (2±0%)	44	89
All	All	129/168 (77%)	126 (98%)	3 (2%)	44	89

All 2 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	35	GLN	2
1	A	53	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 51% for the well-defined parts and 49% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `gen_shifts.str`

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	466
Number of shifts mapped to atoms	466
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 [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 51%, i.e. 360 atoms were assigned a chemical shift out of a possible 706. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	93/231 (40%)	93/93 (100%)	0/92 (0%)	0/46 (0%)
Sidechain	242/424 (57%)	242/267 (91%)	0/125 (0%)	0/32 (0%)
Aromatic	25/51 (49%)	25/25 (100%)	0/25 (0%)	0/1 (0%)
Overall	360/706 (51%)	360/385 (94%)	0/242 (0%)	0/79 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 49%, i.e. 466 atoms were assigned a chemical shift out of a possible 947. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	122/321 (38%)	122/130 (94%)	0/128 (0%)	0/63 (0%)
Sidechain	319/575 (55%)	319/364 (88%)	0/169 (0%)	0/42 (0%)
Aromatic	25/51 (49%)	25/25 (100%)	0/25 (0%)	0/1 (0%)
Overall	466/947 (49%)	466/519 (90%)	0/322 (0%)	0/106 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

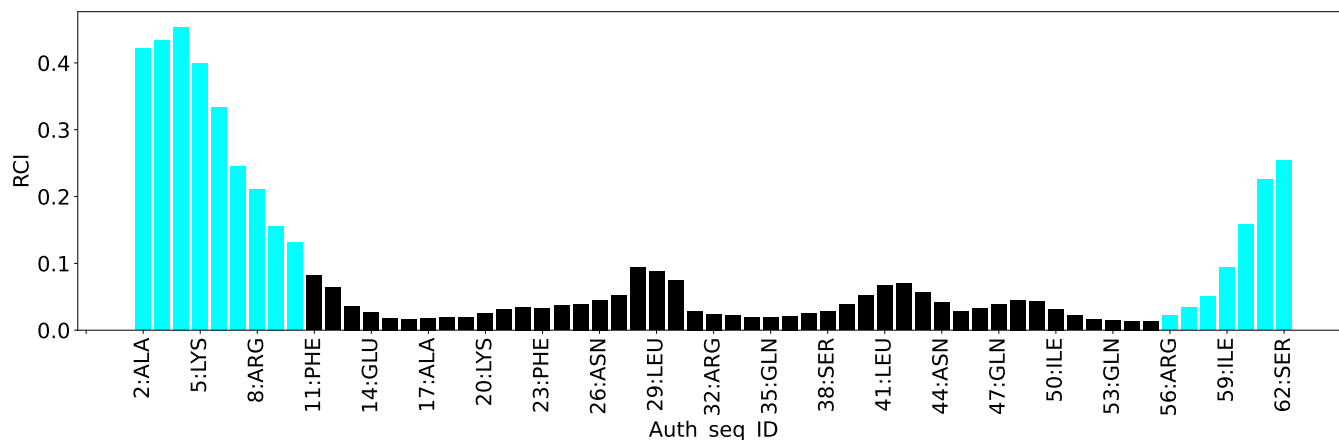
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	55	GLU	HG2	0.15	1.24 – 3.30	-10.3
1	A	55	GLU	HG3	0.20	1.20 – 3.30	-9.8
1	A	55	GLU	HB2	0.06	1.00 – 3.05	-9.6
1	A	55	GLU	HB3	0.32	0.95 – 3.05	-8.0

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1915
Intra-residue ($ i-j =0$)	432
Sequential ($ i-j =1$)	441
Medium range ($ i-j >1$ and $ i-j <5$)	525
Long range ($ i-j \geq 5$)	517
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	29.5
Number of long range restraints per residue ¹	8.0

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)	99.7	0.2
0.2-0.5 (Medium)	172.7	0.5
>0.5 (Large)	102.3	4.34

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

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

9 Distance violation analysis ⓘ

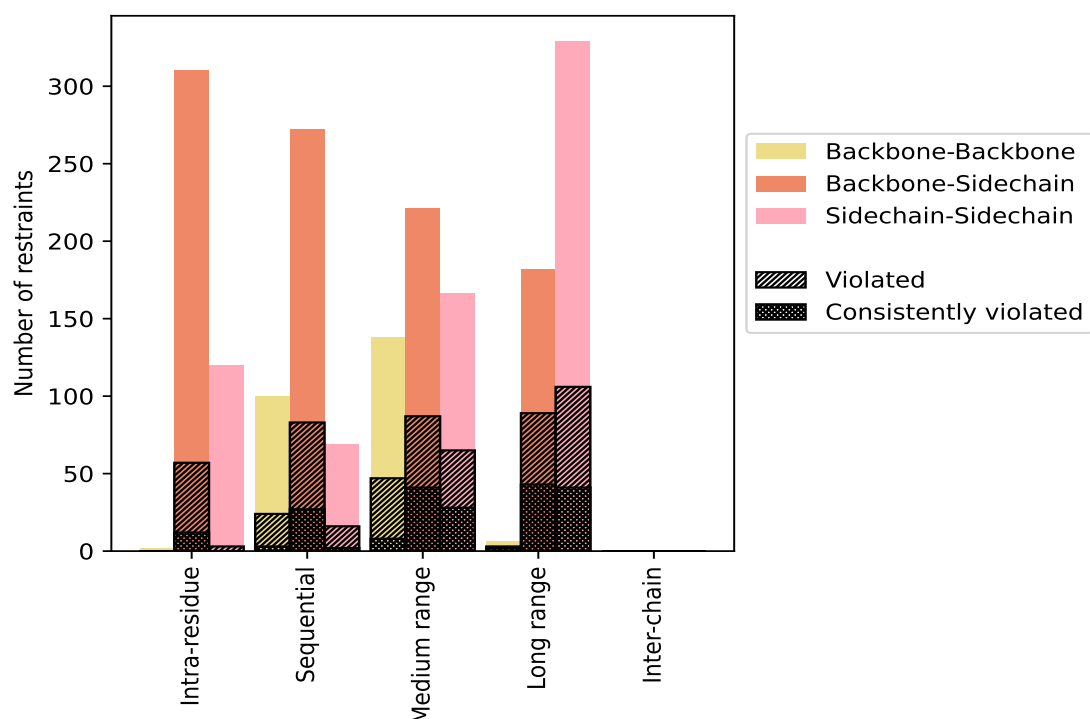
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	432	22.6	60	13.9	3.1	12	2.8	0.6
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	310	16.2	57	18.4	3.0	12	3.9	0.6
Sidechain-Sidechain	120	6.3	3	2.5	0.2	0	0.0	0.0
Sequential ($ i-j =1$)	441	23.0	123	27.9	6.4	32	7.3	1.7
Backbone-Backbone	100	5.2	24	24.0	1.3	3	3.0	0.2
Backbone-Sidechain	272	14.2	83	30.5	4.3	27	9.9	1.4
Sidechain-Sidechain	69	3.6	16	23.2	0.8	2	2.9	0.1
Medium range ($ i-j >1$ & $ i-j <5$)	525	27.4	199	37.9	10.4	77	14.7	4.0
Backbone-Backbone	138	7.2	47	34.1	2.5	8	5.8	0.4
Backbone-Sidechain	221	11.5	87	39.4	4.5	41	18.6	2.1
Sidechain-Sidechain	166	8.7	65	39.2	3.4	28	16.9	1.5
Long range ($ i-j \geq 5$)	517	27.0	198	38.3	10.3	86	16.6	4.5
Backbone-Backbone	6	0.3	3	50.0	0.2	2	33.3	0.1
Backbone-Sidechain	182	9.5	89	48.9	4.6	43	23.6	2.2
Sidechain-Sidechain	329	17.2	106	32.2	5.5	41	12.5	2.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1915	100.0	580	30.3	30.3	207	10.8	10.8
Backbone-Backbone	246	12.8	74	30.1	3.9	13	5.3	0.7
Backbone-Sidechain	985	51.4	316	32.1	16.5	123	12.5	6.4
Sidechain-Sidechain	684	35.7	190	27.8	9.9	71	10.4	3.7

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](#)

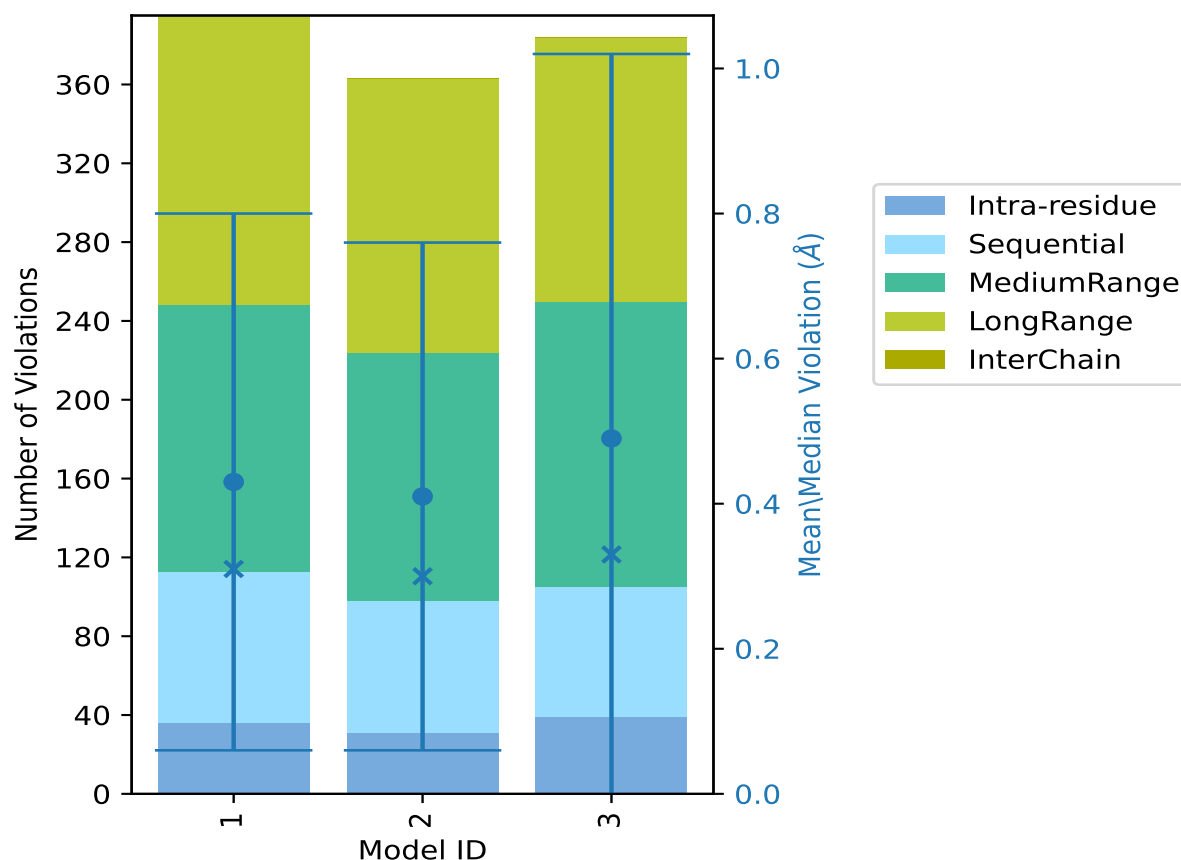
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	36	77	135	147	0	395	0.43	2.73	0.37	0.31
2	31	67	126	139	0	363	0.41	2.71	0.35	0.3
3	39	66	145	134	0	384	0.49	4.34	0.53	0.33

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](#)

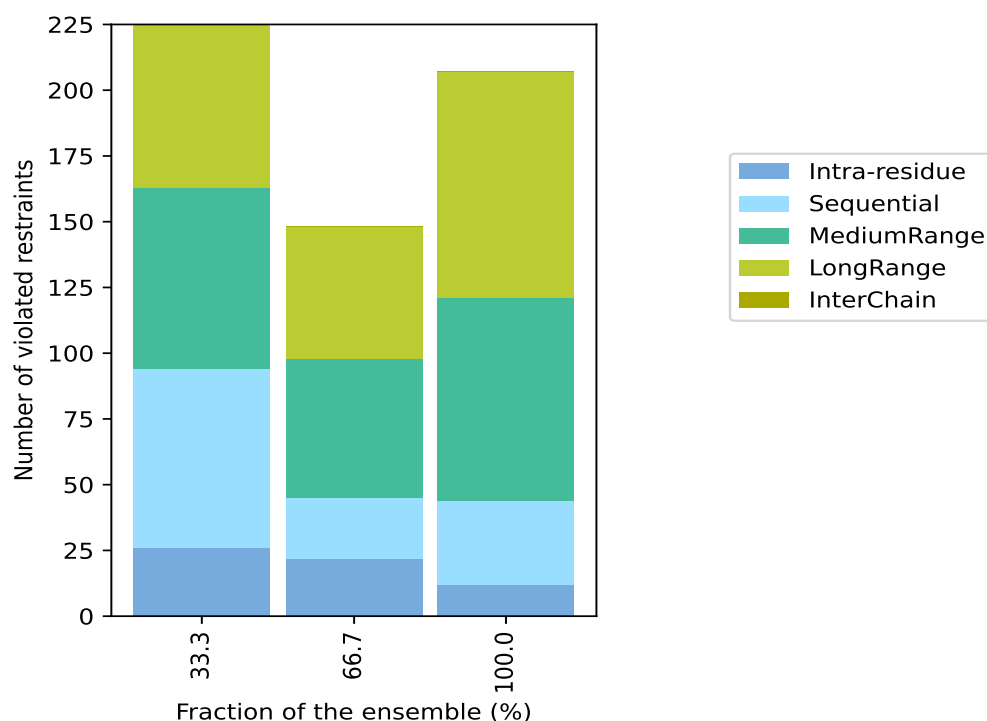
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1335(IR:372, SQ:318, MR:326, LR:319, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
26	68	69	62	0	225	1	33.3
22	23	53	50	0	148	2	66.7
12	32	77	86	0	207	3	100.0

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

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

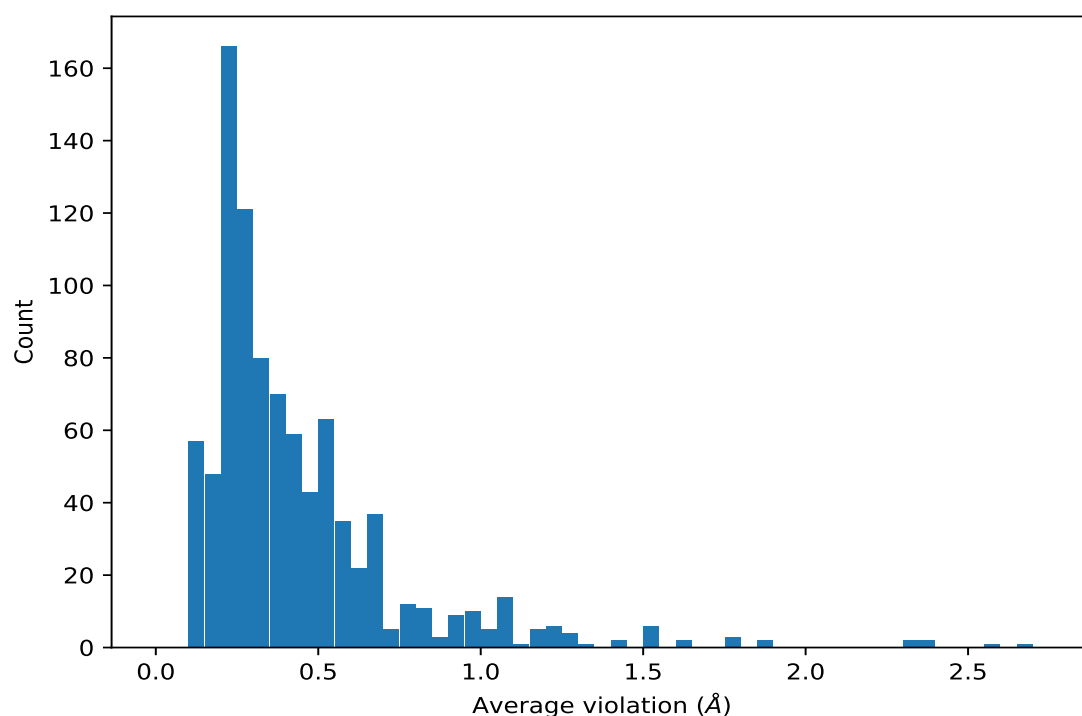
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,519)	1:44:A:ASN:HD21	1:46:A:ALA:HA	3	2.56	0.22	2.71
(1,1219)	1:11:A:PHE:HD1	1:41:A:LEU:HG	3	2.38	0.05	2.4
(1,1219)	1:11:A:PHE:HD2	1:41:A:LEU:HG	3	2.38	0.05	2.4
(1,1856)	1:51:A:TRP:HD1	1:54:A:ASN:HD21	3	2.34	1.61	2.28
(1,1856)	1:51:A:TRP:HD1	1:54:A:ASN:HD22	3	2.34	1.61	2.28
(1,1209)	1:29:A:LEU:HB3	1:49:A:LYS:HA	3	1.79	0.18	1.79
(1,990)	1:29:A:LEU:HG	1:33:A:ARG:HB2	3	1.64	0.11	1.65
(1,990)	1:29:A:LEU:HG	1:33:A:ARG:HB3	3	1.64	0.11	1.65
(1,1508)	1:9:A:THR:HG21	1:58:A:LYS:HG2	3	1.53	0.25	1.51
(1,1508)	1:9:A:THR:HG21	1:58:A:LYS:HG3	3	1.53	0.25	1.51
(1,1508)	1:9:A:THR:HG22	1:58:A:LYS:HG2	3	1.53	0.25	1.51
(1,1508)	1:9:A:THR:HG22	1:58:A:LYS:HG3	3	1.53	0.25	1.51
(1,1508)	1:9:A:THR:HG23	1:58:A:LYS:HG2	3	1.53	0.25	1.51
(1,1508)	1:9:A:THR:HG23	1:58:A:LYS:HG3	3	1.53	0.25	1.51
(1,1576)	1:15:A:GLN:HG2	1:41:A:LEU:HG	3	1.43	0.04	1.43
(1,1576)	1:15:A:GLN:HG3	1:41:A:LEU:HG	3	1.43	0.04	1.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,292)	1:12:A:SER:H	1:16:A:LEU:HB3	3	1.32	0.33	1.29
(1,64)	1:18:A:ARG:H	1:41:A:LEU:HG	3	1.28	0.3	1.11
(1,1387)	1:54:A:ASN:HD22	1:55:A:GLU:HA	3	1.27	1.04	0.66
(1,1409)	1:34:A:ARG:HG2	1:45:A:GLU:HG2	3	1.26	0.25	1.19
(1,1409)	1:34:A:ARG:HG3	1:45:A:GLU:HG2	3	1.26	0.25	1.19
(1,1216)	1:15:A:GLN:HE21	1:43:A:LEU:HB2	3	1.24	0.25	1.21
(1,1216)	1:15:A:GLN:HE21	1:43:A:LEU:HB3	3	1.24	0.25	1.21
(1,690)	1:11:A:PHE:HZ	1:49:A:LYS:H	3	1.24	0.14	1.19
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD21	3	1.21	0.23	1.29
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD22	3	1.21	0.23	1.29
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD23	3	1.21	0.23	1.29
(1,1877)	1:54:A:ASN:HD21	1:55:A:GLU:HA	3	1.18	0.58	0.94
(1,1877)	1:54:A:ASN:HD22	1:55:A:GLU:HA	3	1.18	0.58	0.94
(1,819)	1:54:A:ASN:HD21	1:55:A:GLU:HA	3	1.12	0.41	1.13
(1,1469)	1:15:A:GLN:HE21	1:43:A:LEU:H	3	1.08	0.23	1.01
(1,805)	1:34:A:ARG:HD2	1:48:A:ILE:HA	3	1.07	0.07	1.08
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD21	3	1.06	0.26	1.11
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD22	3	1.06	0.26	1.11
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD23	3	1.06	0.26	1.11
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD21	3	1.06	0.26	1.11
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD22	3	1.06	0.26	1.11
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD23	3	1.06	0.26	1.11
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD11	3	1.06	0.17	1.12
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD12	3	1.06	0.17	1.12
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD13	3	1.06	0.17	1.12
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD21	3	1.06	0.17	1.12
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD22	3	1.06	0.17	1.12
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD23	3	1.06	0.17	1.12
(1,1386)	1:15:A:GLN:HA	1:41:A:LEU:HG	3	1.04	0.01	1.03
(1,1325)	1:28:A:TYR:HA	1:53:A:GLN:HG3	3	1.01	0.12	1.04
(1,1190)	1:19:A:LEU:HD11	1:41:A:LEU:HG	3	1.01	0.03	1.02
(1,1190)	1:19:A:LEU:HD12	1:41:A:LEU:HG	3	1.01	0.03	1.02
(1,1190)	1:19:A:LEU:HD13	1:41:A:LEU:HG	3	1.01	0.03	1.02
(1,1136)	1:38:A:SER:HB3	1:48:A:ILE:HG12	3	0.98	0.08	0.93
(1,1136)	1:38:A:SER:HB3	1:48:A:ILE:HG13	3	0.98	0.08	0.93
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD21	3	0.98	0.08	1.01
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD22	3	0.98	0.08	1.01
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD23	3	0.98	0.08	1.01
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD11	3	0.97	0.22	1.1
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD12	3	0.97	0.22	1.1
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD13	3	0.97	0.22	1.1
(1,408)	1:18:A:ARG:HE	1:19:A:LEU:H	3	0.97	0.03	0.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1460)	1:19:A:LEU:HA	1:41:A:LEU:HG	3	0.96	0.03	0.98
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD11	3	0.94	0.4	1.2
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD12	3	0.94	0.4	1.2
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD13	3	0.94	0.4	1.2
(1,1302)	1:18:A:ARG:HB2	1:41:A:LEU:H	3	0.94	0.19	0.89
(1,1302)	1:18:A:ARG:HB3	1:41:A:LEU:H	3	0.94	0.19	0.89
(1,1360)	1:51:A:TRP:HE3	1:55:A:GLU:HG3	3	0.93	0.09	0.91
(1,282)	1:16:A:LEU:HA	1:20:A:LYS:HD2	3	0.92	0.08	0.86
(1,282)	1:16:A:LEU:HA	1:20:A:LYS:HD3	3	0.92	0.08	0.86
(1,1177)	1:19:A:LEU:HG	1:37:A:LEU:HB2	3	0.89	0.21	0.75
(1,1574)	1:15:A:GLN:HG2	1:41:A:LEU:H	3	0.88	0.2	0.93
(1,1574)	1:15:A:GLN:HG3	1:41:A:LEU:H	3	0.88	0.2	0.93
(1,1884)	1:56:A:ARG:H	1:58:A:LYS:HG2	3	0.84	0.32	0.93
(1,1884)	1:56:A:ARG:H	1:58:A:LYS:HG3	3	0.84	0.32	0.93
(1,850)	1:34:A:ARG:HE	1:49:A:LYS:HA	3	0.84	0.19	0.74
(1,610)	1:20:A:LYS:HG2	1:23:A:PHE:HD1	3	0.83	0.15	0.87
(1,610)	1:20:A:LYS:HG2	1:23:A:PHE:HD2	3	0.83	0.15	0.87
(1,610)	1:20:A:LYS:HG3	1:23:A:PHE:HD1	3	0.83	0.15	0.87
(1,610)	1:20:A:LYS:HG3	1:23:A:PHE:HD2	3	0.83	0.15	0.87
(1,807)	1:34:A:ARG:HD3	1:48:A:ILE:HA	3	0.8	0.1	0.75
(1,263)	1:15:A:GLN:HE21	1:42:A:GLY:H	3	0.78	0.19	0.65
(1,727)	1:23:A:PHE:HZ	1:27:A:ARG:HD2	3	0.77	0.15	0.73
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD21	3	0.76	0.06	0.74
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD22	3	0.76	0.06	0.74
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD23	3	0.76	0.06	0.74
(1,1107)	1:29:A:LEU:HG	1:34:A:ARG:H	3	0.76	0.01	0.77
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD11	3	0.76	0.19	0.87
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD12	3	0.76	0.19	0.87
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD13	3	0.76	0.19	0.87
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD21	3	0.76	0.19	0.87
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD22	3	0.76	0.19	0.87
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD23	3	0.76	0.19	0.87
(1,321)	1:44:A:ASN:HD21	1:45:A:GLU:H	3	0.74	0.15	0.66
(1,542)	1:44:A:ASN:HD21	1:47:A:GLN:HG2	3	0.74	0.37	0.61
(1,1286)	1:19:A:LEU:HA	1:20:A:LYS:HD2	3	0.73	0.17	0.84
(1,1286)	1:19:A:LEU:HA	1:20:A:LYS:HD3	3	0.73	0.17	0.84
(1,931)	1:27:A:ARG:HB2	1:56:A:ARG:HD3	3	0.71	0.18	0.75
(1,1630)	1:20:A:LYS:HG2	1:24:A:ASN:HD21	3	0.7	0.38	0.5
(1,1630)	1:20:A:LYS:HG2	1:24:A:ASN:HD22	3	0.7	0.38	0.5
(1,1630)	1:20:A:LYS:HG3	1:24:A:ASN:HD21	3	0.7	0.38	0.5
(1,1630)	1:20:A:LYS:HG3	1:24:A:ASN:HD22	3	0.7	0.38	0.5
(1,1910)	1:61:A:LYS:H	1:61:A:LYS:HD2	3	0.7	0.13	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1910)	1:61:A:LYS:H	1:61:A:LYS:HD3	3	0.7	0.13	0.68
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD11	3	0.69	0.09	0.66
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD12	3	0.69	0.09	0.66
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD13	3	0.69	0.09	0.66
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD21	3	0.69	0.09	0.66
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD22	3	0.69	0.09	0.66
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD23	3	0.69	0.09	0.66
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD11	3	0.69	0.11	0.66
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD12	3	0.69	0.11	0.66
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD13	3	0.69	0.11	0.66
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD11	3	0.67	0.27	0.55
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD12	3	0.67	0.27	0.55
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD13	3	0.67	0.27	0.55
(1,716)	1:50:A:ILE:HD11	1:53:A:GLN:HE21	3	0.67	0.23	0.78
(1,716)	1:50:A:ILE:HD12	1:53:A:GLN:HE21	3	0.67	0.23	0.78
(1,716)	1:50:A:ILE:HD13	1:53:A:GLN:HE21	3	0.67	0.23	0.78
(1,1817)	1:41:A:LEU:HD11	1:43:A:LEU:H	3	0.67	0.06	0.69
(1,1817)	1:41:A:LEU:HD12	1:43:A:LEU:H	3	0.67	0.06	0.69
(1,1817)	1:41:A:LEU:HD13	1:43:A:LEU:H	3	0.67	0.06	0.69
(1,1817)	1:41:A:LEU:HD21	1:43:A:LEU:H	3	0.67	0.06	0.69
(1,1817)	1:41:A:LEU:HD22	1:43:A:LEU:H	3	0.67	0.06	0.69
(1,1817)	1:41:A:LEU:HD23	1:43:A:LEU:H	3	0.67	0.06	0.69
(1,1173)	1:19:A:LEU:HD21	1:37:A:LEU:HG	3	0.67	0.2	0.69
(1,1173)	1:19:A:LEU:HD22	1:37:A:LEU:HG	3	0.67	0.2	0.69
(1,1173)	1:19:A:LEU:HD23	1:37:A:LEU:HG	3	0.67	0.2	0.69
(1,798)	1:45:A:GLU:HA	1:49:A:LYS:HA	3	0.66	0.07	0.64
(1,312)	1:43:A:LEU:HG	1:44:A:ASN:H	3	0.66	0.13	0.58
(1,1284)	1:33:A:ARG:HD3	1:36:A:GLN:HB2	3	0.65	0.49	0.4
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD11	3	0.65	0.34	0.68
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD12	3	0.65	0.34	0.68
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD13	3	0.65	0.34	0.68
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD11	3	0.64	0.36	0.63
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD12	3	0.64	0.36	0.63
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD13	3	0.64	0.36	0.63
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD21	3	0.64	0.36	0.63
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD22	3	0.64	0.36	0.63
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD23	3	0.64	0.36	0.63
(1,833)	1:30:A:THR:H	1:33:A:ARG:HD2	3	0.64	0.08	0.65
(1,1116)	1:59:A:ILE:HG21	1:61:A:LYS:HG3	3	0.63	0.15	0.71
(1,1116)	1:59:A:ILE:HG22	1:61:A:LYS:HG3	3	0.63	0.15	0.71
(1,1116)	1:59:A:ILE:HG23	1:61:A:LYS:HG3	3	0.63	0.15	0.71
(1,1179)	1:43:A:LEU:HG	1:47:A:GLN:HB2	3	0.61	0.03	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,813)	1:15:A:GLN:HA	1:41:A:LEU:HA	3	0.61	0.36	0.41
(1,1824)	1:43:A:LEU:HD11	1:45:A:GLU:HA	3	0.61	0.09	0.55
(1,1824)	1:43:A:LEU:HD12	1:45:A:GLU:HA	3	0.61	0.09	0.55
(1,1824)	1:43:A:LEU:HD13	1:45:A:GLU:HA	3	0.61	0.09	0.55
(1,1824)	1:43:A:LEU:HD21	1:45:A:GLU:HA	3	0.61	0.09	0.55
(1,1824)	1:43:A:LEU:HD22	1:45:A:GLU:HA	3	0.61	0.09	0.55
(1,1824)	1:43:A:LEU:HD23	1:45:A:GLU:HA	3	0.61	0.09	0.55
(1,903)	1:34:A:ARG:HD3	1:49:A:LYS:HD3	3	0.6	0.08	0.63
(1,1062)	1:52:A:PHE:HB3	1:55:A:GLU:HB2	3	0.6	0.02	0.6
(1,1628)	1:20:A:LYS:HA	1:24:A:ASN:HD21	3	0.59	0.24	0.5
(1,1628)	1:20:A:LYS:HA	1:24:A:ASN:HD22	3	0.59	0.24	0.5
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD11	3	0.59	0.11	0.58
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD12	3	0.59	0.11	0.58
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD13	3	0.59	0.11	0.58
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD21	3	0.59	0.11	0.58
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD22	3	0.59	0.11	0.58
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD23	3	0.59	0.11	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD11	3	0.59	0.11	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD12	3	0.59	0.11	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD13	3	0.59	0.11	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD21	3	0.59	0.11	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD22	3	0.59	0.11	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD23	3	0.59	0.11	0.58
(1,1397)	1:19:A:LEU:HD11	1:48:A:ILE:H	3	0.59	0.33	0.72
(1,1397)	1:19:A:LEU:HD12	1:48:A:ILE:H	3	0.59	0.33	0.72
(1,1397)	1:19:A:LEU:HD13	1:48:A:ILE:H	3	0.59	0.33	0.72
(1,775)	1:55:A:GLU:HA	1:58:A:LYS:HG2	3	0.58	0.32	0.43
(1,297)	1:11:A:PHE:HE1	1:12:A:SER:H	3	0.58	0.21	0.45
(1,297)	1:11:A:PHE:HE2	1:12:A:SER:H	3	0.58	0.21	0.45
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD11	3	0.57	0.05	0.6
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD12	3	0.57	0.05	0.6
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD13	3	0.57	0.05	0.6
(1,1634)	1:21:A:ARG:HA	1:24:A:ASN:HB2	3	0.57	0.08	0.56
(1,1634)	1:21:A:ARG:HA	1:24:A:ASN:HB3	3	0.57	0.08	0.56
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD11	3	0.56	0.1	0.62
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD12	3	0.56	0.1	0.62
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD13	3	0.56	0.1	0.62
(1,1012)	1:30:A:THR:HG21	1:32:A:ARG:H	3	0.55	0.16	0.44
(1,1012)	1:30:A:THR:HG22	1:32:A:ARG:H	3	0.55	0.16	0.44
(1,1012)	1:30:A:THR:HG23	1:32:A:ARG:H	3	0.55	0.16	0.44
(1,1839)	1:49:A:LYS:HA	1:49:A:LYS:HD2	3	0.55	0.08	0.59
(1,1839)	1:49:A:LYS:HA	1:49:A:LYS:HD3	3	0.55	0.08	0.59

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,790)	1:51:A:TRP:HA	1:55:A:GLU:HA	3	0.54	0.3	0.65
(1,770)	1:52:A:PHE:HA	1:55:A:GLU:HG3	3	0.54	0.21	0.52
(1,1013)	1:41:A:LEU:H	1:43:A:LEU:HG	3	0.53	0.09	0.47
(1,1364)	1:30:A:THR:H	1:33:A:ARG:HE	3	0.53	0.09	0.59
(1,1328)	1:28:A:TYR:HE1	1:53:A:GLN:HG3	3	0.53	0.26	0.38
(1,1328)	1:28:A:TYR:HE2	1:53:A:GLN:HG3	3	0.53	0.26	0.38
(1,1131)	1:34:A:ARG:HA	1:48:A:ILE:HG12	3	0.52	0.19	0.62
(1,1131)	1:34:A:ARG:HA	1:48:A:ILE:HG13	3	0.52	0.19	0.62
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG21	3	0.51	0.15	0.53
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG22	3	0.51	0.15	0.53
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG23	3	0.51	0.15	0.53
(1,295)	1:13:A:SER:H	1:17:A:ALA:H	3	0.5	0.05	0.47
(1,764)	1:24:A:ASN:H	1:51:A:TRP:HZ3	3	0.5	0.07	0.55
(1,1233)	1:30:A:THR:HG21	1:34:A:ARG:H	3	0.5	0.09	0.53
(1,1233)	1:30:A:THR:HG22	1:34:A:ARG:H	3	0.5	0.09	0.53
(1,1233)	1:30:A:THR:HG23	1:34:A:ARG:H	3	0.5	0.09	0.53
(1,1740)	1:30:A:THR:HA	1:31:A:GLU:HG2	3	0.5	0.22	0.5
(1,1740)	1:30:A:THR:HA	1:31:A:GLU:HG3	3	0.5	0.22	0.5
(1,1180)	1:38:A:SER:HA	1:43:A:LEU:HG	3	0.49	0.16	0.51
(1,1494)	1:6:A:ARG:HB2	1:7:A:PRO:HG2	3	0.49	0.11	0.44
(1,1494)	1:6:A:ARG:HB3	1:7:A:PRO:HG2	3	0.49	0.11	0.44
(1,1366)	1:56:A:ARG:H	1:56:A:ARG:HE	3	0.49	0.09	0.46
(1,346)	1:44:A:ASN:H	1:47:A:GLN:HA	3	0.48	0.1	0.55
(1,1815)	1:41:A:LEU:HD11	1:42:A:GLY:H	3	0.48	0.06	0.46
(1,1815)	1:41:A:LEU:HD12	1:42:A:GLY:H	3	0.48	0.06	0.46
(1,1815)	1:41:A:LEU:HD13	1:42:A:GLY:H	3	0.48	0.06	0.46
(1,1815)	1:41:A:LEU:HD21	1:42:A:GLY:H	3	0.48	0.06	0.46
(1,1815)	1:41:A:LEU:HD22	1:42:A:GLY:H	3	0.48	0.06	0.46
(1,1815)	1:41:A:LEU:HD23	1:42:A:GLY:H	3	0.48	0.06	0.46
(1,1367)	1:44:A:ASN:HD21	1:47:A:GLN:H	3	0.48	0.16	0.46
(1,1712)	1:29:A:LEU:HD11	1:33:A:ARG:HD2	3	0.48	0.14	0.39
(1,1712)	1:29:A:LEU:HD11	1:33:A:ARG:HD3	3	0.48	0.14	0.39
(1,1712)	1:29:A:LEU:HD12	1:33:A:ARG:HD2	3	0.48	0.14	0.39
(1,1712)	1:29:A:LEU:HD12	1:33:A:ARG:HD3	3	0.48	0.14	0.39
(1,1712)	1:29:A:LEU:HD13	1:33:A:ARG:HD2	3	0.48	0.14	0.39
(1,1712)	1:29:A:LEU:HD13	1:33:A:ARG:HD3	3	0.48	0.14	0.39
(1,1712)	1:29:A:LEU:HD21	1:33:A:ARG:HD2	3	0.48	0.14	0.39
(1,1712)	1:29:A:LEU:HD21	1:33:A:ARG:HD3	3	0.48	0.14	0.39
(1,1712)	1:29:A:LEU:HD22	1:33:A:ARG:HD2	3	0.48	0.14	0.39
(1,1712)	1:29:A:LEU:HD22	1:33:A:ARG:HD3	3	0.48	0.14	0.39
(1,1712)	1:29:A:LEU:HD23	1:33:A:ARG:HD2	3	0.48	0.14	0.39
(1,1712)	1:29:A:LEU:HD23	1:33:A:ARG:HD3	3	0.48	0.14	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,695)	1:11:A:PHE:HZ	1:47:A:GLN:H	3	0.47	0.1	0.49
(1,1057)	1:19:A:LEU:HD21	1:48:A:ILE:H	3	0.46	0.22	0.52
(1,1057)	1:19:A:LEU:HD22	1:48:A:ILE:H	3	0.46	0.22	0.52
(1,1057)	1:19:A:LEU:HD23	1:48:A:ILE:H	3	0.46	0.22	0.52
(1,1160)	1:38:A:SER:H	1:48:A:ILE:HG12	3	0.46	0.16	0.56
(1,1160)	1:38:A:SER:H	1:48:A:ILE:HG13	3	0.46	0.16	0.56
(1,1690)	1:27:A:ARG:H	1:56:A:ARG:HD2	3	0.46	0.04	0.46
(1,1690)	1:27:A:ARG:H	1:56:A:ARG:HD3	3	0.46	0.04	0.46
(1,665)	1:23:A:PHE:HD1	1:55:A:GLU:HA	3	0.45	0.03	0.44
(1,665)	1:23:A:PHE:HD2	1:55:A:GLU:HA	3	0.45	0.03	0.44
(1,834)	1:30:A:THR:H	1:34:A:ARG:HD3	3	0.45	0.08	0.42
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD11	3	0.45	0.17	0.36
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD12	3	0.45	0.17	0.36
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD13	3	0.45	0.17	0.36
(1,888)	1:53:A:GLN:HG2	1:54:A:ASN:HA	3	0.45	0.09	0.41
(1,341)	1:12:A:SER:HB3	1:14:A:GLU:H	3	0.44	0.27	0.28
(1,526)	1:23:A:PHE:HZ	1:55:A:GLU:H	3	0.44	0.11	0.39
(1,269)	1:11:A:PHE:H	1:11:A:PHE:HE1	3	0.43	0.15	0.5
(1,269)	1:11:A:PHE:H	1:11:A:PHE:HE2	3	0.43	0.15	0.5
(1,1738)	1:29:A:LEU:HD11	1:53:A:GLN:H	3	0.42	0.2	0.37
(1,1738)	1:29:A:LEU:HD12	1:53:A:GLN:H	3	0.42	0.2	0.37
(1,1738)	1:29:A:LEU:HD13	1:53:A:GLN:H	3	0.42	0.2	0.37
(1,1738)	1:29:A:LEU:HD21	1:53:A:GLN:H	3	0.42	0.2	0.37
(1,1738)	1:29:A:LEU:HD22	1:53:A:GLN:H	3	0.42	0.2	0.37
(1,1738)	1:29:A:LEU:HD23	1:53:A:GLN:H	3	0.42	0.2	0.37
(1,832)	1:53:A:GLN:HA	1:53:A:GLN:HE22	3	0.42	0.11	0.38
(1,364)	1:48:A:ILE:HB	1:52:A:PHE:H	3	0.42	0.07	0.37
(1,1734)	1:29:A:LEU:HD11	1:52:A:PHE:HA	3	0.42	0.07	0.45
(1,1734)	1:29:A:LEU:HD12	1:52:A:PHE:HA	3	0.42	0.07	0.45
(1,1734)	1:29:A:LEU:HD13	1:52:A:PHE:HA	3	0.42	0.07	0.45
(1,1734)	1:29:A:LEU:HD21	1:52:A:PHE:HA	3	0.42	0.07	0.45
(1,1734)	1:29:A:LEU:HD22	1:52:A:PHE:HA	3	0.42	0.07	0.45
(1,1734)	1:29:A:LEU:HD23	1:52:A:PHE:HA	3	0.42	0.07	0.45
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD11	3	0.42	0.12	0.4
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD12	3	0.42	0.12	0.4
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD13	3	0.42	0.12	0.4
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD21	3	0.42	0.12	0.4
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD22	3	0.42	0.12	0.4
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD23	3	0.42	0.12	0.4
(1,1463)	1:11:A:PHE:HB3	1:15:A:GLN:H	3	0.41	0.15	0.32
(1,1343)	1:22:A:GLU:HG2	1:37:A:LEU:H	3	0.4	0.12	0.42
(1,1343)	1:22:A:GLU:HG3	1:37:A:LEU:H	3	0.4	0.12	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1418)	1:11:A:PHE:HB2	1:16:A:LEU:HB3	3	0.4	0.09	0.39
(1,1669)	1:24:A:ASN:HD21	1:25:A:GLU:HA	3	0.4	0.12	0.36
(1,1669)	1:24:A:ASN:HD22	1:25:A:GLU:HA	3	0.4	0.12	0.36
(1,108)	1:10:A:ALA:H	1:47:A:GLN:HE22	3	0.4	0.12	0.48
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD21	3	0.4	0.14	0.5
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD22	3	0.4	0.14	0.5
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD23	3	0.4	0.14	0.5
(1,544)	1:42:A:GLY:H	1:43:A:LEU:HA	3	0.4	0.1	0.41
(1,1373)	1:23:A:PHE:HE1	1:27:A:ARG:HD2	3	0.4	0.21	0.35
(1,1373)	1:23:A:PHE:HE2	1:27:A:ARG:HD2	3	0.4	0.21	0.35
(1,1064)	1:19:A:LEU:HD21	1:22:A:GLU:HB3	3	0.39	0.11	0.38
(1,1064)	1:19:A:LEU:HD22	1:22:A:GLU:HB3	3	0.39	0.11	0.38
(1,1064)	1:19:A:LEU:HD23	1:22:A:GLU:HB3	3	0.39	0.11	0.38
(1,1640)	1:21:A:ARG:HB2	1:24:A:ASN:HB2	3	0.39	0.08	0.34
(1,1640)	1:21:A:ARG:HB2	1:24:A:ASN:HB3	3	0.39	0.08	0.34
(1,1640)	1:21:A:ARG:HB3	1:24:A:ASN:HB2	3	0.39	0.08	0.34
(1,1640)	1:21:A:ARG:HB3	1:24:A:ASN:HB3	3	0.39	0.08	0.34
(1,1482)	1:11:A:PHE:HB2	1:16:A:LEU:HB2	3	0.39	0.14	0.38
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD11	3	0.39	0.13	0.31
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD12	3	0.39	0.13	0.31
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD13	3	0.39	0.13	0.31
(1,1911)	1:61:A:LYS:HA	1:61:A:LYS:HD2	3	0.39	0.06	0.35
(1,1911)	1:61:A:LYS:HA	1:61:A:LYS:HD3	3	0.39	0.06	0.35
(1,627)	1:9:A:THR:HA	1:11:A:PHE:HE1	3	0.39	0.08	0.35
(1,627)	1:9:A:THR:HA	1:11:A:PHE:HE2	3	0.39	0.08	0.35
(1,561)	1:22:A:GLU:HB2	1:52:A:PHE:HD1	3	0.38	0.02	0.38
(1,561)	1:22:A:GLU:HB2	1:52:A:PHE:HD2	3	0.38	0.02	0.38
(1,789)	1:19:A:LEU:HA	1:22:A:GLU:HA	3	0.38	0.04	0.36
(1,1609)	1:18:A:ARG:HD2	1:22:A:GLU:H	3	0.38	0.26	0.25
(1,1609)	1:18:A:ARG:HD3	1:22:A:GLU:H	3	0.38	0.26	0.25
(1,102)	1:29:A:LEU:HA	1:33:A:ARG:HE	3	0.38	0.18	0.33
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG21	3	0.38	0.06	0.34
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG22	3	0.38	0.06	0.34
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG23	3	0.38	0.06	0.34
(1,661)	1:23:A:PHE:HB3	1:51:A:TRP:HE3	3	0.38	0.09	0.38
(1,717)	1:50:A:ILE:HG21	1:51:A:TRP:HD1	3	0.38	0.01	0.37
(1,717)	1:50:A:ILE:HG22	1:51:A:TRP:HD1	3	0.38	0.01	0.37
(1,717)	1:50:A:ILE:HG23	1:51:A:TRP:HD1	3	0.38	0.01	0.37
(1,490)	1:9:A:THR:HG21	1:11:A:PHE:H	3	0.37	0.07	0.42
(1,490)	1:9:A:THR:HG22	1:11:A:PHE:H	3	0.37	0.07	0.42
(1,490)	1:9:A:THR:HG23	1:11:A:PHE:H	3	0.37	0.07	0.42
(1,381)	1:18:A:ARG:HE	1:22:A:GLU:HB2	3	0.37	0.03	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1404)	1:34:A:ARG:HD3	1:45:A:GLU:HA	3	0.37	0.12	0.36
(1,1047)	1:29:A:LEU:HD21	1:52:A:PHE:HB2	3	0.36	0.12	0.35
(1,1047)	1:29:A:LEU:HD22	1:52:A:PHE:HB2	3	0.36	0.12	0.35
(1,1047)	1:29:A:LEU:HD23	1:52:A:PHE:HB2	3	0.36	0.12	0.35
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD21	3	0.36	0.21	0.33
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD22	3	0.36	0.21	0.33
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD23	3	0.36	0.21	0.33
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD11	3	0.36	0.14	0.39
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD12	3	0.36	0.14	0.39
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD13	3	0.36	0.14	0.39
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD21	3	0.36	0.14	0.39
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD22	3	0.36	0.14	0.39
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD23	3	0.36	0.14	0.39
(1,1008)	1:20:A:LYS:H	1:20:A:LYS:HD2	3	0.36	0.09	0.32
(1,1008)	1:20:A:LYS:H	1:20:A:LYS:HD3	3	0.36	0.09	0.32
(1,405)	1:29:A:LEU:HA	1:34:A:ARG:H	3	0.36	0.03	0.37
(1,291)	1:34:A:ARG:HB3	1:45:A:GLU:H	3	0.35	0.18	0.47
(1,880)	1:22:A:GLU:HG2	1:37:A:LEU:HA	3	0.35	0.26	0.19
(1,880)	1:22:A:GLU:HG3	1:37:A:LEU:HA	3	0.35	0.26	0.19
(1,1213)	1:28:A:TYR:HA	1:29:A:LEU:HB3	3	0.35	0.08	0.38
(1,1731)	1:29:A:LEU:HD11	1:49:A:LYS:HB2	3	0.34	0.1	0.28
(1,1731)	1:29:A:LEU:HD12	1:49:A:LYS:HB2	3	0.34	0.1	0.28
(1,1731)	1:29:A:LEU:HD13	1:49:A:LYS:HB2	3	0.34	0.1	0.28
(1,1731)	1:29:A:LEU:HD21	1:49:A:LYS:HB2	3	0.34	0.1	0.28
(1,1731)	1:29:A:LEU:HD22	1:49:A:LYS:HB2	3	0.34	0.1	0.28
(1,1731)	1:29:A:LEU:HD23	1:49:A:LYS:HB2	3	0.34	0.1	0.28
(1,867)	1:38:A:SER:HB3	1:45:A:GLU:HA	3	0.34	0.16	0.41
(1,1540)	1:12:A:SER:HB2	1:15:A:GLN:H	3	0.34	0.16	0.23
(1,1540)	1:12:A:SER:HB3	1:15:A:GLN:H	3	0.34	0.16	0.23
(1,34)	1:16:A:LEU:HD11	1:51:A:TRP:HH2	3	0.33	0.15	0.3
(1,34)	1:16:A:LEU:HD12	1:51:A:TRP:HH2	3	0.33	0.15	0.3
(1,34)	1:16:A:LEU:HD13	1:51:A:TRP:HH2	3	0.33	0.15	0.3
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB1	3	0.33	0.07	0.34
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB2	3	0.33	0.07	0.34
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB3	3	0.33	0.07	0.34
(1,1252)	1:34:A:ARG:HB3	1:48:A:ILE:HB	3	0.33	0.03	0.35
(1,674)	1:23:A:PHE:HE1	1:56:A:ARG:HA	3	0.33	0.08	0.37
(1,674)	1:23:A:PHE:HE2	1:56:A:ARG:HA	3	0.33	0.08	0.37
(1,818)	1:48:A:ILE:HA	1:51:A:TRP:HD1	3	0.33	0.12	0.36
(1,1287)	1:19:A:LEU:HA	1:22:A:GLU:HB3	3	0.33	0.03	0.32
(1,1514)	1:11:A:PHE:HB2	1:15:A:GLN:HB2	3	0.33	0.02	0.33
(1,1514)	1:11:A:PHE:HB2	1:15:A:GLN:HB3	3	0.33	0.02	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1403)	1:23:A:PHE:HD1	1:27:A:ARG:H	3	0.32	0.11	0.35
(1,1403)	1:23:A:PHE:HD2	1:27:A:ARG:H	3	0.32	0.11	0.35
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG21	3	0.32	0.16	0.41
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG22	3	0.32	0.16	0.41
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG23	3	0.32	0.16	0.41
(1,1666)	1:24:A:ASN:HB2	1:25:A:GLU:H	3	0.32	0.04	0.34
(1,1666)	1:24:A:ASN:HB3	1:25:A:GLU:H	3	0.32	0.04	0.34
(1,1818)	1:41:A:LEU:HD11	1:43:A:LEU:HG	3	0.31	0.06	0.31
(1,1818)	1:41:A:LEU:HD12	1:43:A:LEU:HG	3	0.31	0.06	0.31
(1,1818)	1:41:A:LEU:HD13	1:43:A:LEU:HG	3	0.31	0.06	0.31
(1,1818)	1:41:A:LEU:HD21	1:43:A:LEU:HG	3	0.31	0.06	0.31
(1,1818)	1:41:A:LEU:HD22	1:43:A:LEU:HG	3	0.31	0.06	0.31
(1,1818)	1:41:A:LEU:HD23	1:43:A:LEU:HG	3	0.31	0.06	0.31
(1,293)	1:11:A:PHE:HE1	1:51:A:TRP:HE1	3	0.31	0.02	0.32
(1,293)	1:11:A:PHE:HE2	1:51:A:TRP:HE1	3	0.31	0.02	0.32
(1,697)	1:11:A:PHE:HZ	1:51:A:TRP:HE1	3	0.31	0.14	0.24
(1,1042)	1:29:A:LEU:HD11	1:30:A:THR:H	3	0.31	0.05	0.29
(1,1042)	1:29:A:LEU:HD12	1:30:A:THR:H	3	0.31	0.05	0.29
(1,1042)	1:29:A:LEU:HD13	1:30:A:THR:H	3	0.31	0.05	0.29
(1,1186)	1:11:A:PHE:HE1	1:43:A:LEU:HG	3	0.31	0.04	0.31
(1,1186)	1:11:A:PHE:HE2	1:43:A:LEU:HG	3	0.31	0.04	0.31
(1,559)	1:29:A:LEU:H	1:52:A:PHE:HD1	3	0.3	0.2	0.17
(1,559)	1:29:A:LEU:H	1:52:A:PHE:HD2	3	0.3	0.2	0.17
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD21	3	0.3	0.22	0.16
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD22	3	0.3	0.22	0.16
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD23	3	0.3	0.22	0.16
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD21	3	0.3	0.22	0.16
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD22	3	0.3	0.22	0.16
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD23	3	0.3	0.22	0.16
(1,1225)	1:37:A:LEU:HG	1:52:A:PHE:HE1	3	0.3	0.12	0.3
(1,1225)	1:37:A:LEU:HG	1:52:A:PHE:HE2	3	0.3	0.12	0.3
(1,1406)	1:51:A:TRP:HB2	1:52:A:PHE:HA	3	0.3	0.03	0.31
(1,891)	1:18:A:ARG:HB2	1:37:A:LEU:HA	3	0.29	0.14	0.34
(1,891)	1:18:A:ARG:HB3	1:37:A:LEU:HA	3	0.29	0.14	0.34
(1,1174)	1:19:A:LEU:HD21	1:41:A:LEU:HG	3	0.29	0.1	0.24
(1,1174)	1:19:A:LEU:HD22	1:41:A:LEU:HG	3	0.29	0.1	0.24
(1,1174)	1:19:A:LEU:HD23	1:41:A:LEU:HG	3	0.29	0.1	0.24
(1,583)	1:29:A:LEU:HB3	1:52:A:PHE:HD1	3	0.28	0.03	0.3
(1,583)	1:29:A:LEU:HB3	1:52:A:PHE:HD2	3	0.28	0.03	0.3
(1,347)	1:31:A:GLU:H	1:32:A:ARG:HA	3	0.28	0.13	0.32
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB1	3	0.27	0.04	0.28
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB2	3	0.27	0.04	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB3	3	0.27	0.04	0.28
(1,693)	1:24:A:ASN:H	1:52:A:PHE:HZ	3	0.27	0.09	0.31
(1,189)	1:44:A:ASN:HA	1:44:A:ASN:HD21	3	0.26	0.07	0.22
(1,270)	1:11:A:PHE:HA	1:11:A:PHE:HE1	3	0.26	0.07	0.21
(1,270)	1:11:A:PHE:HA	1:11:A:PHE:HE2	3	0.26	0.07	0.21
(1,654)	1:48:A:ILE:HG21	1:51:A:TRP:HE3	3	0.26	0.04	0.25
(1,654)	1:48:A:ILE:HG22	1:51:A:TRP:HE3	3	0.26	0.04	0.25
(1,654)	1:48:A:ILE:HG23	1:51:A:TRP:HE3	3	0.26	0.04	0.25
(1,1802)	1:38:A:SER:HB2	1:48:A:ILE:HG12	3	0.26	0.12	0.22
(1,1802)	1:38:A:SER:HB2	1:48:A:ILE:HG13	3	0.26	0.12	0.22
(1,1802)	1:38:A:SER:HB3	1:48:A:ILE:HG12	3	0.26	0.12	0.22
(1,1802)	1:38:A:SER:HB3	1:48:A:ILE:HG13	3	0.26	0.12	0.22
(1,508)	1:19:A:LEU:HD11	1:52:A:PHE:HD1	3	0.25	0.06	0.27
(1,508)	1:19:A:LEU:HD11	1:52:A:PHE:HD2	3	0.25	0.06	0.27
(1,508)	1:19:A:LEU:HD12	1:52:A:PHE:HD1	3	0.25	0.06	0.27
(1,508)	1:19:A:LEU:HD12	1:52:A:PHE:HD2	3	0.25	0.06	0.27
(1,508)	1:19:A:LEU:HD13	1:52:A:PHE:HD1	3	0.25	0.06	0.27
(1,508)	1:19:A:LEU:HD13	1:52:A:PHE:HD2	3	0.25	0.06	0.27
(1,705)	1:23:A:PHE:HZ	1:55:A:GLU:HB2	3	0.25	0.09	0.19
(1,372)	1:44:A:ASN:H	1:46:A:ALA:H	3	0.24	0.05	0.23
(1,1038)	1:29:A:LEU:HD11	1:33:A:ARG:HA	3	0.24	0.0	0.24
(1,1038)	1:29:A:LEU:HD12	1:33:A:ARG:HA	3	0.24	0.0	0.24
(1,1038)	1:29:A:LEU:HD13	1:33:A:ARG:HA	3	0.24	0.0	0.24
(1,707)	1:29:A:LEU:HD21	1:51:A:TRP:HE3	3	0.24	0.1	0.21
(1,707)	1:29:A:LEU:HD22	1:51:A:TRP:HE3	3	0.24	0.1	0.21
(1,707)	1:29:A:LEU:HD23	1:51:A:TRP:HE3	3	0.24	0.1	0.21
(1,1431)	1:45:A:GLU:HB3	1:47:A:GLN:H	3	0.24	0.02	0.23
(1,1363)	1:18:A:ARG:H	1:21:A:ARG:H	3	0.23	0.08	0.19
(1,1341)	1:56:A:ARG:H	1:56:A:ARG:HD2	3	0.23	0.05	0.2
(1,523)	1:29:A:LEU:HA	1:52:A:PHE:HD1	3	0.23	0.08	0.27
(1,523)	1:29:A:LEU:HA	1:52:A:PHE:HD2	3	0.23	0.08	0.27
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD11	3	0.22	0.09	0.22
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD12	3	0.22	0.09	0.22
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD13	3	0.22	0.09	0.22
(1,1477)	1:51:A:TRP:HB3	1:52:A:PHE:HA	3	0.22	0.05	0.2
(1,1480)	1:19:A:LEU:HG	1:51:A:TRP:HE3	3	0.22	0.06	0.23
(1,779)	1:55:A:GLU:HA	1:58:A:LYS:HB3	3	0.22	0.08	0.16
(1,1687)	1:26:A:ASN:HD21	1:27:A:ARG:H	3	0.22	0.07	0.22
(1,1687)	1:26:A:ASN:HD22	1:27:A:ARG:H	3	0.22	0.07	0.22
(1,426)	1:19:A:LEU:HD21	1:20:A:LYS:H	3	0.22	0.05	0.2
(1,426)	1:19:A:LEU:HD22	1:20:A:LYS:H	3	0.22	0.05	0.2
(1,426)	1:19:A:LEU:HD23	1:20:A:LYS:H	3	0.22	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,609)	1:11:A:PHE:HD1	1:16:A:LEU:HB2	3	0.22	0.12	0.15
(1,609)	1:11:A:PHE:HD2	1:16:A:LEU:HB2	3	0.22	0.12	0.15
(1,720)	1:23:A:PHE:HD1	1:27:A:ARG:HB2	3	0.22	0.04	0.22
(1,720)	1:23:A:PHE:HD2	1:27:A:ARG:HB2	3	0.22	0.04	0.22
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD21	3	0.22	0.05	0.23
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD22	3	0.22	0.05	0.23
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD23	3	0.22	0.05	0.23
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD21	3	0.22	0.05	0.23
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD22	3	0.22	0.05	0.23
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD23	3	0.22	0.05	0.23
(1,575)	1:29:A:LEU:HG	1:30:A:THR:H	3	0.22	0.08	0.22
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB1	3	0.2	0.01	0.2
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB2	3	0.2	0.01	0.2
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB3	3	0.2	0.01	0.2
(1,1043)	1:29:A:LEU:HD11	1:33:A:ARG:HE	3	0.2	0.07	0.16
(1,1043)	1:29:A:LEU:HD12	1:33:A:ARG:HE	3	0.2	0.07	0.16
(1,1043)	1:29:A:LEU:HD13	1:33:A:ARG:HE	3	0.2	0.07	0.16
(1,410)	1:19:A:LEU:HD11	1:20:A:LYS:H	3	0.2	0.02	0.19
(1,410)	1:19:A:LEU:HD12	1:20:A:LYS:H	3	0.2	0.02	0.19
(1,410)	1:19:A:LEU:HD13	1:20:A:LYS:H	3	0.2	0.02	0.19
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD21	3	0.19	0.1	0.12
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD22	3	0.19	0.1	0.12
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD23	3	0.19	0.1	0.12
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD21	3	0.19	0.1	0.12
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD22	3	0.19	0.1	0.12
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD23	3	0.19	0.1	0.12
(1,1142)	1:9:A:THR:HG21	1:10:A:ALA:HA	3	0.19	0.04	0.2
(1,1142)	1:9:A:THR:HG22	1:10:A:ALA:HA	3	0.19	0.04	0.2
(1,1142)	1:9:A:THR:HG23	1:10:A:ALA:HA	3	0.19	0.04	0.2
(1,517)	1:15:A:GLN:H	1:16:A:LEU:HA	3	0.17	0.05	0.18
(1,633)	1:33:A:ARG:H	1:35:A:GLN:H	3	0.17	0.04	0.18
(1,1357)	1:16:A:LEU:HA	1:20:A:LYS:HB2	3	0.17	0.05	0.14
(1,694)	1:23:A:PHE:HE1	1:28:A:TYR:H	3	0.17	0.02	0.16
(1,694)	1:23:A:PHE:HE2	1:28:A:TYR:H	3	0.17	0.02	0.16
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD11	3	0.16	0.05	0.13
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD12	3	0.16	0.05	0.13
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD13	3	0.16	0.05	0.13
(1,1606)	1:18:A:ARG:HD2	1:19:A:LEU:H	3	0.16	0.02	0.17
(1,1606)	1:18:A:ARG:HD3	1:19:A:LEU:H	3	0.16	0.02	0.17
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD11	3	0.14	0.04	0.12
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD12	3	0.14	0.04	0.12
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD13	3	0.14	0.04	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,365)	1:50:A:ILE:HB	1:52:A:PHE:H	3	0.13	0.03	0.12
(1,1391)	1:51:A:TRP:HA	1:54:A:ASN:HD22	2	2.68	1.0	2.68
(1,1855)	1:51:A:TRP:HB2	1:54:A:ASN:HD21	2	1.88	1.51	1.88
(1,1855)	1:51:A:TRP:HB2	1:54:A:ASN:HD22	2	1.88	1.51	1.88
(1,1854)	1:51:A:TRP:HA	1:54:A:ASN:HD21	2	1.78	1.33	1.78
(1,1854)	1:51:A:TRP:HA	1:54:A:ASN:HD22	2	1.78	1.33	1.78
(1,1185)	1:50:A:ILE:HG21	1:53:A:GLN:HE21	2	1.19	0.1	1.19
(1,1185)	1:50:A:ILE:HG22	1:53:A:GLN:HE21	2	1.19	0.1	1.19
(1,1185)	1:50:A:ILE:HG23	1:53:A:GLN:HE21	2	1.19	0.1	1.19
(1,737)	1:9:A:THR:HA	1:51:A:TRP:HD1	2	0.94	0.0	0.94
(1,1148)	1:51:A:TRP:HH2	1:59:A:ILE:HD11	2	0.85	0.12	0.85
(1,1148)	1:51:A:TRP:HH2	1:59:A:ILE:HD12	2	0.85	0.12	0.85
(1,1148)	1:51:A:TRP:HH2	1:59:A:ILE:HD13	2	0.85	0.12	0.85
(1,869)	1:58:A:LYS:HA	1:58:A:LYS:HE3	2	0.7	0.01	0.7
(1,151)	1:35:A:GLN:HE22	1:36:A:GLN:HB3	2	0.64	0.03	0.64
(1,1056)	1:43:A:LEU:HD11	1:47:A:GLN:HE22	2	0.63	0.27	0.63
(1,1056)	1:43:A:LEU:HD12	1:47:A:GLN:HE22	2	0.63	0.27	0.63
(1,1056)	1:43:A:LEU:HD13	1:47:A:GLN:HE22	2	0.63	0.27	0.63
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD11	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD12	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD13	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD21	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD22	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD23	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD11	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD12	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD13	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD21	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD22	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD23	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD11	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD12	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD13	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD21	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD22	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD23	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD11	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD12	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD13	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD21	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD22	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD23	2	0.54	0.15	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD11	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD12	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD13	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD21	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD22	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD23	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD11	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD12	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD13	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD21	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD22	2	0.54	0.15	0.54
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD23	2	0.54	0.15	0.54
(1,1245)	1:37:A:LEU:HB2	1:48:A:ILE:HG12	2	0.52	0.04	0.52
(1,1245)	1:37:A:LEU:HB2	1:48:A:ILE:HG13	2	0.52	0.04	0.52
(1,1828)	1:43:A:LEU:HD11	1:48:A:ILE:H	2	0.5	0.01	0.5
(1,1828)	1:43:A:LEU:HD12	1:48:A:ILE:H	2	0.5	0.01	0.5
(1,1828)	1:43:A:LEU:HD13	1:48:A:ILE:H	2	0.5	0.01	0.5
(1,1828)	1:43:A:LEU:HD21	1:48:A:ILE:H	2	0.5	0.01	0.5
(1,1828)	1:43:A:LEU:HD22	1:48:A:ILE:H	2	0.5	0.01	0.5
(1,1828)	1:43:A:LEU:HD23	1:48:A:ILE:H	2	0.5	0.01	0.5
(1,315)	1:44:A:ASN:H	1:47:A:GLN:HB3	2	0.5	0.1	0.5
(1,762)	1:20:A:LYS:HA	1:51:A:TRP:HZ3	2	0.45	0.02	0.45
(1,905)	1:9:A:THR:HG21	1:51:A:TRP:HB2	2	0.45	0.17	0.45
(1,905)	1:9:A:THR:HG22	1:51:A:TRP:HB2	2	0.45	0.17	0.45
(1,905)	1:9:A:THR:HG23	1:51:A:TRP:HB2	2	0.45	0.17	0.45
(1,564)	1:47:A:GLN:HA	1:47:A:GLN:HE21	2	0.43	0.1	0.43
(1,530)	1:28:A:TYR:HD1	1:56:A:ARG:HE	2	0.42	0.04	0.42
(1,530)	1:28:A:TYR:HD2	1:56:A:ARG:HE	2	0.42	0.04	0.42
(1,1748)	1:32:A:ARG:HA	1:32:A:ARG:HD2	2	0.42	0.14	0.42
(1,1748)	1:32:A:ARG:HA	1:32:A:ARG:HD3	2	0.42	0.14	0.42
(1,1389)	1:35:A:GLN:HE21	1:36:A:GLN:HG2	2	0.42	0.28	0.42
(1,1389)	1:35:A:GLN:HE21	1:36:A:GLN:HG3	2	0.42	0.28	0.42
(1,1365)	1:38:A:SER:H	1:42:A:GLY:H	2	0.41	0.18	0.41
(1,1110)	1:19:A:LEU:HD21	1:41:A:LEU:HD21	2	0.4	0.16	0.4
(1,1110)	1:19:A:LEU:HD21	1:41:A:LEU:HD22	2	0.4	0.16	0.4
(1,1110)	1:19:A:LEU:HD21	1:41:A:LEU:HD23	2	0.4	0.16	0.4
(1,1110)	1:19:A:LEU:HD22	1:41:A:LEU:HD21	2	0.4	0.16	0.4
(1,1110)	1:19:A:LEU:HD22	1:41:A:LEU:HD22	2	0.4	0.16	0.4
(1,1110)	1:19:A:LEU:HD22	1:41:A:LEU:HD23	2	0.4	0.16	0.4
(1,1110)	1:19:A:LEU:HD23	1:41:A:LEU:HD21	2	0.4	0.16	0.4
(1,1110)	1:19:A:LEU:HD23	1:41:A:LEU:HD22	2	0.4	0.16	0.4
(1,1110)	1:19:A:LEU:HD23	1:41:A:LEU:HD23	2	0.4	0.16	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,415)	1:5:A:LYS:HA	1:6:A:ARG:H	2	0.4	0.24	0.4
(1,898)	1:21:A:ARG:HD2	1:22:A:GLU:H	2	0.4	0.12	0.4
(1,898)	1:21:A:ARG:HD3	1:22:A:GLU:H	2	0.4	0.12	0.4
(1,1345)	1:20:A:LYS:HE2	1:51:A:TRP:HE1	2	0.4	0.26	0.4
(1,1345)	1:20:A:LYS:HE3	1:51:A:TRP:HE1	2	0.4	0.26	0.4
(1,1585)	1:16:A:LEU:HD11	1:18:A:ARG:H	2	0.39	0.16	0.39
(1,1585)	1:16:A:LEU:HD12	1:18:A:ARG:H	2	0.39	0.16	0.39
(1,1585)	1:16:A:LEU:HD13	1:18:A:ARG:H	2	0.39	0.16	0.39
(1,1585)	1:16:A:LEU:HD21	1:18:A:ARG:H	2	0.39	0.16	0.39
(1,1585)	1:16:A:LEU:HD22	1:18:A:ARG:H	2	0.39	0.16	0.39
(1,1585)	1:16:A:LEU:HD23	1:18:A:ARG:H	2	0.39	0.16	0.39
(1,1790)	1:37:A:LEU:HD11	1:51:A:TRP:HB3	2	0.39	0.13	0.39
(1,1790)	1:37:A:LEU:HD12	1:51:A:TRP:HB3	2	0.39	0.13	0.39
(1,1790)	1:37:A:LEU:HD13	1:51:A:TRP:HB3	2	0.39	0.13	0.39
(1,1790)	1:37:A:LEU:HD21	1:51:A:TRP:HB3	2	0.39	0.13	0.39
(1,1790)	1:37:A:LEU:HD22	1:51:A:TRP:HB3	2	0.39	0.13	0.39
(1,1790)	1:37:A:LEU:HD23	1:51:A:TRP:HB3	2	0.39	0.13	0.39
(1,753)	1:20:A:LYS:H	1:51:A:TRP:HZ2	2	0.38	0.1	0.38
(1,422)	1:61:A:LYS:H	1:62:A:SER:HB2	2	0.38	0.04	0.38
(1,422)	1:61:A:LYS:H	1:62:A:SER:HB3	2	0.38	0.04	0.38
(1,1847)	1:50:A:ILE:H	1:53:A:GLN:HE21	2	0.38	0.26	0.38
(1,1847)	1:50:A:ILE:H	1:53:A:GLN:HE22	2	0.38	0.26	0.38
(1,1699)	1:27:A:ARG:HG2	1:56:A:ARG:HD2	2	0.38	0.01	0.38
(1,1699)	1:27:A:ARG:HG2	1:56:A:ARG:HD3	2	0.38	0.01	0.38
(1,1699)	1:27:A:ARG:HG3	1:56:A:ARG:HD2	2	0.38	0.01	0.38
(1,1699)	1:27:A:ARG:HG3	1:56:A:ARG:HD3	2	0.38	0.01	0.38
(1,1301)	1:25:A:GLU:HG2	1:26:A:ASN:H	2	0.37	0.11	0.37
(1,394)	1:44:A:ASN:HD21	1:46:A:ALA:H	2	0.35	0.09	0.35
(1,1050)	1:38:A:SER:HA	1:43:A:LEU:HD11	2	0.34	0.06	0.34
(1,1050)	1:38:A:SER:HA	1:43:A:LEU:HD12	2	0.34	0.06	0.34
(1,1050)	1:38:A:SER:HA	1:43:A:LEU:HD13	2	0.34	0.06	0.34
(1,463)	1:51:A:TRP:HE3	1:53:A:GLN:H	2	0.34	0.02	0.34
(1,760)	1:24:A:ASN:H	1:51:A:TRP:HH2	2	0.34	0.05	0.34
(1,1157)	1:50:A:ILE:HG21	1:53:A:GLN:HE22	2	0.34	0.02	0.34
(1,1157)	1:50:A:ILE:HG22	1:53:A:GLN:HE22	2	0.34	0.02	0.34
(1,1157)	1:50:A:ILE:HG23	1:53:A:GLN:HE22	2	0.34	0.02	0.34
(1,1354)	1:11:A:PHE:HB2	1:12:A:SER:HA	2	0.34	0.02	0.34
(1,820)	1:23:A:PHE:HZ	1:55:A:GLU:HA	2	0.33	0.13	0.33
(1,262)	1:15:A:GLN:H	1:15:A:GLN:HE21	2	0.32	0.09	0.32
(1,1135)	1:37:A:LEU:HA	1:48:A:ILE:HG12	2	0.32	0.2	0.32
(1,1135)	1:37:A:LEU:HA	1:48:A:ILE:HG13	2	0.32	0.2	0.32
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD11	2	0.32	0.16	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD12	2	0.32	0.16	0.32
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD13	2	0.32	0.16	0.32
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD21	2	0.32	0.16	0.32
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD22	2	0.32	0.16	0.32
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD23	2	0.32	0.16	0.32
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD11	2	0.32	0.16	0.32
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD12	2	0.32	0.16	0.32
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD13	2	0.32	0.16	0.32
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD21	2	0.32	0.16	0.32
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD22	2	0.32	0.16	0.32
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD23	2	0.32	0.16	0.32
(1,294)	1:12:A:SER:H	1:16:A:LEU:H	2	0.32	0.14	0.32
(1,35)	1:20:A:LYS:HG2	1:51:A:TRP:HH2	2	0.32	0.1	0.32
(1,35)	1:20:A:LYS:HG3	1:51:A:TRP:HH2	2	0.32	0.1	0.32
(1,488)	1:29:A:LEU:HB3	1:34:A:ARG:HE	2	0.32	0.1	0.32
(1,689)	1:23:A:PHE:HE1	1:27:A:ARG:H	2	0.32	0.07	0.32
(1,689)	1:23:A:PHE:HE2	1:27:A:ARG:H	2	0.32	0.07	0.32
(1,319)	1:44:A:ASN:HD22	1:45:A:GLU:H	2	0.32	0.01	0.32
(1,1172)	1:19:A:LEU:HD11	1:48:A:ILE:HG21	2	0.3	0.0	0.3
(1,1172)	1:19:A:LEU:HD11	1:48:A:ILE:HG22	2	0.3	0.0	0.3
(1,1172)	1:19:A:LEU:HD11	1:48:A:ILE:HG23	2	0.3	0.0	0.3
(1,1172)	1:19:A:LEU:HD12	1:48:A:ILE:HG21	2	0.3	0.0	0.3
(1,1172)	1:19:A:LEU:HD12	1:48:A:ILE:HG22	2	0.3	0.0	0.3
(1,1172)	1:19:A:LEU:HD12	1:48:A:ILE:HG23	2	0.3	0.0	0.3
(1,1172)	1:19:A:LEU:HD13	1:48:A:ILE:HG21	2	0.3	0.0	0.3
(1,1172)	1:19:A:LEU:HD13	1:48:A:ILE:HG22	2	0.3	0.0	0.3
(1,1172)	1:19:A:LEU:HD13	1:48:A:ILE:HG23	2	0.3	0.0	0.3
(1,1662)	1:24:A:ASN:H	1:24:A:ASN:HD21	2	0.3	0.06	0.3
(1,1662)	1:24:A:ASN:H	1:24:A:ASN:HD22	2	0.3	0.06	0.3
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD11	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD12	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD13	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD21	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD22	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD23	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD11	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD12	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD13	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD21	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD22	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD23	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD11	2	0.3	0.04	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD12	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD13	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD21	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD22	2	0.3	0.04	0.3
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD23	2	0.3	0.04	0.3
(1,650)	1:23:A:PHE:HE1	1:55:A:GLU:HB2	2	0.29	0.06	0.29
(1,650)	1:23:A:PHE:HE2	1:55:A:GLU:HB2	2	0.29	0.06	0.29
(1,443)	1:38:A:SER:H	1:40:A:GLU:H	2	0.28	0.15	0.28
(1,1256)	1:34:A:ARG:HA	1:48:A:ILE:HB	2	0.28	0.05	0.28
(1,1377)	1:49:A:LYS:HB2	1:50:A:ILE:HA	2	0.28	0.06	0.28
(1,1394)	1:11:A:PHE:HD1	1:16:A:LEU:HB3	2	0.28	0.03	0.28
(1,1394)	1:11:A:PHE:HD2	1:16:A:LEU:HB3	2	0.28	0.03	0.28
(1,1730)	1:29:A:LEU:HD11	1:49:A:LYS:HA	2	0.28	0.18	0.28
(1,1730)	1:29:A:LEU:HD12	1:49:A:LYS:HA	2	0.28	0.18	0.28
(1,1730)	1:29:A:LEU:HD13	1:49:A:LYS:HA	2	0.28	0.18	0.28
(1,1730)	1:29:A:LEU:HD21	1:49:A:LYS:HA	2	0.28	0.18	0.28
(1,1730)	1:29:A:LEU:HD22	1:49:A:LYS:HA	2	0.28	0.18	0.28
(1,1730)	1:29:A:LEU:HD23	1:49:A:LYS:HA	2	0.28	0.18	0.28
(1,20)	1:15:A:GLN:HA	1:15:A:GLN:HE21	2	0.27	0.05	0.27
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD11	2	0.27	0.1	0.27
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD12	2	0.27	0.1	0.27
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD13	2	0.27	0.1	0.27
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD21	2	0.27	0.1	0.27
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD22	2	0.27	0.1	0.27
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD23	2	0.27	0.1	0.27
(1,184)	1:8:A:ARG:HA	1:8:A:ARG:HD2	2	0.26	0.14	0.26
(1,184)	1:8:A:ARG:HA	1:8:A:ARG:HD3	2	0.26	0.14	0.26
(1,1054)	1:19:A:LEU:HD21	1:23:A:PHE:HD1	2	0.26	0.01	0.26
(1,1054)	1:19:A:LEU:HD21	1:23:A:PHE:HD2	2	0.26	0.01	0.26
(1,1054)	1:19:A:LEU:HD22	1:23:A:PHE:HD1	2	0.26	0.01	0.26
(1,1054)	1:19:A:LEU:HD22	1:23:A:PHE:HD2	2	0.26	0.01	0.26
(1,1054)	1:19:A:LEU:HD23	1:23:A:PHE:HD1	2	0.26	0.01	0.26
(1,1054)	1:19:A:LEU:HD23	1:23:A:PHE:HD2	2	0.26	0.01	0.26
(1,1065)	1:19:A:LEU:HD21	1:48:A:ILE:HB	2	0.26	0.16	0.26
(1,1065)	1:19:A:LEU:HD22	1:48:A:ILE:HB	2	0.26	0.16	0.26
(1,1065)	1:19:A:LEU:HD23	1:48:A:ILE:HB	2	0.26	0.16	0.26
(1,1151)	1:15:A:GLN:HE21	1:41:A:LEU:HD21	2	0.26	0.16	0.26
(1,1151)	1:15:A:GLN:HE21	1:41:A:LEU:HD22	2	0.26	0.16	0.26
(1,1151)	1:15:A:GLN:HE21	1:41:A:LEU:HD23	2	0.26	0.16	0.26
(1,666)	1:23:A:PHE:HD1	1:52:A:PHE:HB2	2	0.26	0.0	0.26
(1,666)	1:23:A:PHE:HD2	1:52:A:PHE:HB2	2	0.26	0.0	0.26
(1,755)	1:51:A:TRP:HD1	1:52:A:PHE:H	2	0.26	0.05	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1476)	1:51:A:TRP:HB3	1:52:A:PHE:HB2	2	0.26	0.02	0.26
(1,247)	1:34:A:ARG:HG2	1:49:A:LYS:H	2	0.25	0.01	0.25
(1,247)	1:34:A:ARG:HG3	1:49:A:LYS:H	2	0.25	0.01	0.25
(1,901)	1:6:A:ARG:HD2	1:7:A:PRO:HD3	2	0.25	0.14	0.25
(1,901)	1:6:A:ARG:HD3	1:7:A:PRO:HD3	2	0.25	0.14	0.25
(1,1053)	1:23:A:PHE:HD1	1:55:A:GLU:HB2	2	0.25	0.06	0.25
(1,1053)	1:23:A:PHE:HD2	1:55:A:GLU:HB2	2	0.25	0.06	0.25
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD11	2	0.25	0.06	0.25
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD12	2	0.25	0.06	0.25
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD13	2	0.25	0.06	0.25
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD21	2	0.25	0.06	0.25
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD22	2	0.25	0.06	0.25
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD23	2	0.25	0.06	0.25
(1,1894)	1:58:A:LYS:HA	1:58:A:LYS:HE2	2	0.25	0.01	0.25
(1,1894)	1:58:A:LYS:HA	1:58:A:LYS:HE3	2	0.25	0.01	0.25
(1,16)	1:12:A:SER:H	1:15:A:GLN:H	2	0.24	0.03	0.24
(1,1269)	1:33:A:ARG:HE	1:36:A:GLN:HB3	2	0.24	0.04	0.24
(1,357)	1:44:A:ASN:H	1:47:A:GLN:HG2	2	0.24	0.1	0.24
(1,303)	1:12:A:SER:H	1:15:A:GLN:HB3	2	0.24	0.05	0.24
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD11	2	0.24	0.05	0.24
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD12	2	0.24	0.05	0.24
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD13	2	0.24	0.05	0.24
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD21	2	0.24	0.05	0.24
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD22	2	0.24	0.05	0.24
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD23	2	0.24	0.05	0.24
(1,546)	1:24:A:ASN:H	1:24:A:ASN:HD22	2	0.24	0.04	0.24
(1,1831)	1:43:A:LEU:HD11	1:48:A:ILE:HG21	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD11	1:48:A:ILE:HG22	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD11	1:48:A:ILE:HG23	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD12	1:48:A:ILE:HG21	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD12	1:48:A:ILE:HG22	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD12	1:48:A:ILE:HG23	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD13	1:48:A:ILE:HG21	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD13	1:48:A:ILE:HG22	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD13	1:48:A:ILE:HG23	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD21	1:48:A:ILE:HG21	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD21	1:48:A:ILE:HG22	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD21	1:48:A:ILE:HG23	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD22	1:48:A:ILE:HG21	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD22	1:48:A:ILE:HG22	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD22	1:48:A:ILE:HG23	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD23	1:48:A:ILE:HG21	2	0.24	0.05	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1831)	1:43:A:LEU:HD23	1:48:A:ILE:HG22	2	0.24	0.05	0.24
(1,1831)	1:43:A:LEU:HD23	1:48:A:ILE:HG23	2	0.24	0.05	0.24
(1,300)	1:12:A:SER:H	1:15:A:GLN:HA	2	0.24	0.06	0.24
(1,441)	1:16:A:LEU:H	1:18:A:ARG:H	2	0.24	0.12	0.24
(1,626)	1:11:A:PHE:HE1	1:47:A:GLN:HA	2	0.24	0.02	0.24
(1,626)	1:11:A:PHE:HE2	1:47:A:GLN:HA	2	0.24	0.02	0.24
(1,733)	1:23:A:PHE:HD1	1:56:A:ARG:HA	2	0.24	0.0	0.24
(1,733)	1:23:A:PHE:HD2	1:56:A:ARG:HA	2	0.24	0.0	0.24
(1,1505)	1:8:A:ARG:HB2	1:9:A:THR:HG21	2	0.24	0.12	0.24
(1,1505)	1:8:A:ARG:HB2	1:9:A:THR:HG22	2	0.24	0.12	0.24
(1,1505)	1:8:A:ARG:HB2	1:9:A:THR:HG23	2	0.24	0.12	0.24
(1,1505)	1:8:A:ARG:HB3	1:9:A:THR:HG21	2	0.24	0.12	0.24
(1,1505)	1:8:A:ARG:HB3	1:9:A:THR:HG22	2	0.24	0.12	0.24
(1,1505)	1:8:A:ARG:HB3	1:9:A:THR:HG23	2	0.24	0.12	0.24
(1,563)	1:22:A:GLU:HA	1:52:A:PHE:HE1	2	0.23	0.0	0.23
(1,563)	1:22:A:GLU:HA	1:52:A:PHE:HE2	2	0.23	0.0	0.23
(1,602)	1:16:A:LEU:HB3	1:51:A:TRP:HZ2	2	0.23	0.05	0.23
(1,768)	1:29:A:LEU:HG	1:34:A:ARG:HA	2	0.23	0.09	0.23
(1,899)	1:29:A:LEU:H	1:52:A:PHE:HB2	2	0.23	0.03	0.23
(1,317)	1:45:A:GLU:H	1:46:A:ALA:HA	2	0.23	0.06	0.23
(1,1104)	1:39:A:SER:H	1:48:A:ILE:HD11	2	0.23	0.02	0.23
(1,1104)	1:39:A:SER:H	1:48:A:ILE:HD12	2	0.23	0.02	0.23
(1,1104)	1:39:A:SER:H	1:48:A:ILE:HD13	2	0.23	0.02	0.23
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD11	2	0.23	0.01	0.23
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD12	2	0.23	0.01	0.23
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD13	2	0.23	0.01	0.23
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD21	2	0.23	0.01	0.23
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD22	2	0.23	0.01	0.23
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD23	2	0.23	0.01	0.23
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD11	2	0.23	0.06	0.23
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD12	2	0.23	0.06	0.23
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD13	2	0.23	0.06	0.23
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD21	2	0.23	0.06	0.23
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD22	2	0.23	0.06	0.23
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD23	2	0.23	0.06	0.23
(1,204)	1:41:A:LEU:HB2	1:43:A:LEU:H	2	0.22	0.11	0.22
(1,1319)	1:20:A:LYS:HA	1:23:A:PHE:HB2	2	0.22	0.04	0.22
(1,962)	1:45:A:GLU:HA	1:45:A:GLU:HG2	2	0.22	0.12	0.22
(1,821)	1:23:A:PHE:HB3	1:51:A:TRP:HZ2	2	0.22	0.08	0.22
(1,1049)	1:19:A:LEU:HD21	1:37:A:LEU:HA	2	0.22	0.01	0.22
(1,1049)	1:19:A:LEU:HD22	1:37:A:LEU:HA	2	0.22	0.01	0.22
(1,1049)	1:19:A:LEU:HD23	1:37:A:LEU:HA	2	0.22	0.01	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,407)	1:18:A:ARG:HE	1:41:A:LEU:HD11	2	0.22	0.02	0.22
(1,407)	1:18:A:ARG:HE	1:41:A:LEU:HD12	2	0.22	0.02	0.22
(1,407)	1:18:A:ARG:HE	1:41:A:LEU:HD13	2	0.22	0.02	0.22
(1,1421)	1:52:A:PHE:HA	1:55:A:GLU:HA	2	0.22	0.06	0.22
(1,1788)	1:37:A:LEU:HD11	1:40:A:GLU:HG2	2	0.22	0.04	0.22
(1,1788)	1:37:A:LEU:HD11	1:40:A:GLU:HG3	2	0.22	0.04	0.22
(1,1788)	1:37:A:LEU:HD12	1:40:A:GLU:HG2	2	0.22	0.04	0.22
(1,1788)	1:37:A:LEU:HD12	1:40:A:GLU:HG3	2	0.22	0.04	0.22
(1,1788)	1:37:A:LEU:HD13	1:40:A:GLU:HG2	2	0.22	0.04	0.22
(1,1788)	1:37:A:LEU:HD13	1:40:A:GLU:HG3	2	0.22	0.04	0.22
(1,1788)	1:37:A:LEU:HD21	1:40:A:GLU:HG2	2	0.22	0.04	0.22
(1,1788)	1:37:A:LEU:HD21	1:40:A:GLU:HG3	2	0.22	0.04	0.22
(1,1788)	1:37:A:LEU:HD22	1:40:A:GLU:HG2	2	0.22	0.04	0.22
(1,1788)	1:37:A:LEU:HD22	1:40:A:GLU:HG3	2	0.22	0.04	0.22
(1,1788)	1:37:A:LEU:HD23	1:40:A:GLU:HG2	2	0.22	0.04	0.22
(1,1788)	1:37:A:LEU:HD23	1:40:A:GLU:HG3	2	0.22	0.04	0.22
(1,713)	1:11:A:PHE:HD1	1:16:A:LEU:HD11	2	0.22	0.08	0.22
(1,713)	1:11:A:PHE:HD1	1:16:A:LEU:HD12	2	0.22	0.08	0.22
(1,713)	1:11:A:PHE:HD1	1:16:A:LEU:HD13	2	0.22	0.08	0.22
(1,713)	1:11:A:PHE:HD2	1:16:A:LEU:HD11	2	0.22	0.08	0.22
(1,713)	1:11:A:PHE:HD2	1:16:A:LEU:HD12	2	0.22	0.08	0.22
(1,713)	1:11:A:PHE:HD2	1:16:A:LEU:HD13	2	0.22	0.08	0.22
(1,942)	1:32:A:ARG:HA	1:32:A:ARG:HG3	2	0.22	0.01	0.22
(1,1295)	1:44:A:ASN:HA	1:45:A:GLU:HG2	2	0.22	0.04	0.22
(1,1308)	1:19:A:LEU:HB2	1:22:A:GLU:HG2	2	0.22	0.07	0.22
(1,1308)	1:19:A:LEU:HB2	1:22:A:GLU:HG3	2	0.22	0.07	0.22
(1,1308)	1:19:A:LEU:HB3	1:22:A:GLU:HG2	2	0.22	0.07	0.22
(1,1308)	1:19:A:LEU:HB3	1:22:A:GLU:HG3	2	0.22	0.07	0.22
(1,314)	1:45:A:GLU:H	1:48:A:ILE:HB	2	0.21	0.05	0.21
(1,722)	1:23:A:PHE:HE1	1:27:A:ARG:HB2	2	0.21	0.05	0.21
(1,722)	1:23:A:PHE:HE2	1:27:A:ARG:HB2	2	0.21	0.05	0.21
(1,1355)	1:33:A:ARG:H	1:35:A:GLN:HB3	2	0.21	0.11	0.21
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD11	2	0.21	0.01	0.21
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD12	2	0.21	0.01	0.21
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD13	2	0.21	0.01	0.21
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD21	2	0.21	0.01	0.21
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD22	2	0.21	0.01	0.21
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD23	2	0.21	0.01	0.21
(1,1861)	1:52:A:PHE:HA	1:55:A:GLU:HG2	2	0.21	0.06	0.21
(1,1861)	1:52:A:PHE:HA	1:55:A:GLU:HG3	2	0.21	0.06	0.21
(1,393)	1:18:A:ARG:H	1:20:A:LYS:H	2	0.21	0.0	0.21
(1,644)	1:19:A:LEU:HD11	1:51:A:TRP:HZ2	2	0.2	0.04	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,644)	1:19:A:LEU:HD12	1:51:A:TRP:HZ2	2	0.2	0.04	0.2
(1,644)	1:19:A:LEU:HD13	1:51:A:TRP:HZ2	2	0.2	0.04	0.2
(1,1398)	1:17:A:ALA:H	1:19:A:LEU:HD11	2	0.2	0.1	0.2
(1,1398)	1:17:A:ALA:H	1:19:A:LEU:HD12	2	0.2	0.1	0.2
(1,1398)	1:17:A:ALA:H	1:19:A:LEU:HD13	2	0.2	0.1	0.2
(1,630)	1:51:A:TRP:HH2	1:52:A:PHE:HE1	2	0.2	0.09	0.2
(1,630)	1:51:A:TRP:HH2	1:52:A:PHE:HE2	2	0.2	0.09	0.2
(1,1005)	1:60:A:LYS:H	1:60:A:LYS:HD2	2	0.2	0.03	0.2
(1,1005)	1:60:A:LYS:H	1:60:A:LYS:HD3	2	0.2	0.03	0.2
(1,1141)	1:50:A:ILE:HG21	1:54:A:ASN:HA	2	0.2	0.04	0.2
(1,1141)	1:50:A:ILE:HG22	1:54:A:ASN:HA	2	0.2	0.04	0.2
(1,1141)	1:50:A:ILE:HG23	1:54:A:ASN:HA	2	0.2	0.04	0.2
(1,750)	1:11:A:PHE:HD1	1:15:A:GLN:HE22	2	0.19	0.05	0.19
(1,750)	1:11:A:PHE:HD2	1:15:A:GLN:HE22	2	0.19	0.05	0.19
(1,817)	1:11:A:PHE:HD1	1:15:A:GLN:HA	2	0.19	0.03	0.19
(1,817)	1:11:A:PHE:HD2	1:15:A:GLN:HA	2	0.19	0.03	0.19
(1,1126)	1:48:A:ILE:HG21	1:51:A:TRP:HB2	2	0.19	0.01	0.19
(1,1126)	1:48:A:ILE:HG22	1:51:A:TRP:HB2	2	0.19	0.01	0.19
(1,1126)	1:48:A:ILE:HG23	1:51:A:TRP:HB2	2	0.19	0.01	0.19
(1,1099)	1:11:A:PHE:HD1	1:19:A:LEU:HB2	2	0.18	0.08	0.18
(1,1099)	1:11:A:PHE:HD1	1:19:A:LEU:HB3	2	0.18	0.08	0.18
(1,1099)	1:11:A:PHE:HD2	1:19:A:LEU:HB2	2	0.18	0.08	0.18
(1,1099)	1:11:A:PHE:HD2	1:19:A:LEU:HB3	2	0.18	0.08	0.18
(1,331)	1:23:A:PHE:H	1:24:A:ASN:HA	2	0.18	0.07	0.18
(1,1722)	1:29:A:LEU:HD11	1:37:A:LEU:HB2	2	0.18	0.0	0.18
(1,1722)	1:29:A:LEU:HD12	1:37:A:LEU:HB2	2	0.18	0.0	0.18
(1,1722)	1:29:A:LEU:HD13	1:37:A:LEU:HB2	2	0.18	0.0	0.18
(1,1722)	1:29:A:LEU:HD21	1:37:A:LEU:HB2	2	0.18	0.0	0.18
(1,1722)	1:29:A:LEU:HD22	1:37:A:LEU:HB2	2	0.18	0.0	0.18
(1,1722)	1:29:A:LEU:HD23	1:37:A:LEU:HB2	2	0.18	0.0	0.18
(1,670)	1:48:A:ILE:HA	1:51:A:TRP:HE3	2	0.18	0.0	0.18
(1,1747)	1:32:A:ARG:HA	1:32:A:ARG:HG2	2	0.18	0.02	0.18
(1,1747)	1:32:A:ARG:HA	1:32:A:ARG:HG3	2	0.18	0.02	0.18
(1,838)	1:51:A:TRP:H	1:52:A:PHE:HA	2	0.17	0.04	0.17
(1,839)	1:51:A:TRP:HB2	1:53:A:GLN:H	2	0.17	0.01	0.17
(1,181)	1:8:A:ARG:H	1:8:A:ARG:HB2	2	0.16	0.02	0.16
(1,567)	1:52:A:PHE:H	1:52:A:PHE:HE1	2	0.16	0.0	0.16
(1,567)	1:52:A:PHE:H	1:52:A:PHE:HE2	2	0.16	0.0	0.16
(1,607)	1:43:A:LEU:HB2	1:47:A:GLN:HE22	2	0.16	0.04	0.16
(1,607)	1:43:A:LEU:HB3	1:47:A:GLN:HE22	2	0.16	0.04	0.16
(1,377)	1:37:A:LEU:H	1:40:A:GLU:H	2	0.16	0.02	0.16
(1,910)	1:37:A:LEU:H	1:37:A:LEU:HB3	2	0.15	0.01	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,625)	1:19:A:LEU:HA	1:52:A:PHE:HE1	2	0.15	0.04	0.15
(1,625)	1:19:A:LEU:HA	1:52:A:PHE:HE2	2	0.15	0.04	0.15
(1,398)	1:46:A:ALA:H	1:50:A:ILE:HD11	2	0.15	0.02	0.15
(1,398)	1:46:A:ALA:H	1:50:A:ILE:HD12	2	0.15	0.02	0.15
(1,398)	1:46:A:ALA:H	1:50:A:ILE:HD13	2	0.15	0.02	0.15
(1,1075)	1:47:A:GLN:HB3	1:50:A:ILE:HD11	2	0.15	0.0	0.15
(1,1075)	1:47:A:GLN:HB3	1:50:A:ILE:HD12	2	0.15	0.0	0.15
(1,1075)	1:47:A:GLN:HB3	1:50:A:ILE:HD13	2	0.15	0.0	0.15
(1,202)	1:47:A:GLN:HG2	1:47:A:GLN:HE22	2	0.14	0.04	0.14
(1,1220)	1:11:A:PHE:HD1	1:43:A:LEU:HB2	2	0.14	0.02	0.14
(1,1220)	1:11:A:PHE:HD1	1:43:A:LEU:HB3	2	0.14	0.02	0.14
(1,1220)	1:11:A:PHE:HD2	1:43:A:LEU:HB2	2	0.14	0.02	0.14
(1,1220)	1:11:A:PHE:HD2	1:43:A:LEU:HB3	2	0.14	0.02	0.14
(1,1361)	1:57:A:ALA:H	1:59:A:ILE:H	2	0.14	0.03	0.14
(1,1401)	1:20:A:LYS:H	1:23:A:PHE:HB3	2	0.14	0.0	0.14
(1,950)	1:35:A:GLN:HA	1:35:A:GLN:HG3	2	0.14	0.01	0.14
(1,1082)	1:19:A:LEU:HB2	1:23:A:PHE:HB3	2	0.14	0.01	0.14
(1,1082)	1:19:A:LEU:HB3	1:23:A:PHE:HB3	2	0.14	0.01	0.14
(1,1506)	1:8:A:ARG:HG2	1:9:A:THR:H	2	0.14	0.02	0.14
(1,1506)	1:8:A:ARG:HG3	1:9:A:THR:H	2	0.14	0.02	0.14
(1,709)	1:43:A:LEU:HD21	1:47:A:GLN:HE22	2	0.13	0.0	0.13
(1,709)	1:43:A:LEU:HD22	1:47:A:GLN:HE22	2	0.13	0.0	0.13
(1,709)	1:43:A:LEU:HD23	1:47:A:GLN:HE22	2	0.13	0.0	0.13
(1,1462)	1:41:A:LEU:H	1:42:A:GLY:HA2	2	0.13	0.01	0.13
(1,1708)	1:29:A:LEU:HD11	1:30:A:THR:H	2	0.13	0.01	0.13
(1,1708)	1:29:A:LEU:HD12	1:30:A:THR:H	2	0.13	0.01	0.13
(1,1708)	1:29:A:LEU:HD13	1:30:A:THR:H	2	0.13	0.01	0.13
(1,1708)	1:29:A:LEU:HD21	1:30:A:THR:H	2	0.13	0.01	0.13
(1,1708)	1:29:A:LEU:HD22	1:30:A:THR:H	2	0.13	0.01	0.13
(1,1708)	1:29:A:LEU:HD23	1:30:A:THR:H	2	0.13	0.01	0.13
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD11	2	0.13	0.01	0.13
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD12	2	0.13	0.01	0.13
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD13	2	0.13	0.01	0.13
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD21	2	0.13	0.01	0.13
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD22	2	0.13	0.01	0.13
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD23	2	0.13	0.01	0.13
(1,631)	1:23:A:PHE:HD1	1:55:A:GLU:H	2	0.12	0.01	0.12
(1,631)	1:23:A:PHE:HD2	1:55:A:GLU:H	2	0.12	0.01	0.12
(1,829)	1:51:A:TRP:HB2	1:51:A:TRP:HE3	2	0.12	0.01	0.12
(1,854)	1:37:A:LEU:H	1:38:A:SER:HA	2	0.12	0.01	0.12
(1,164)	1:51:A:TRP:HB3	1:51:A:TRP:HZ3	2	0.12	0.0	0.12
(1,1234)	1:14:A:GLU:H	1:17:A:ALA:HB1	2	0.12	0.0	0.12

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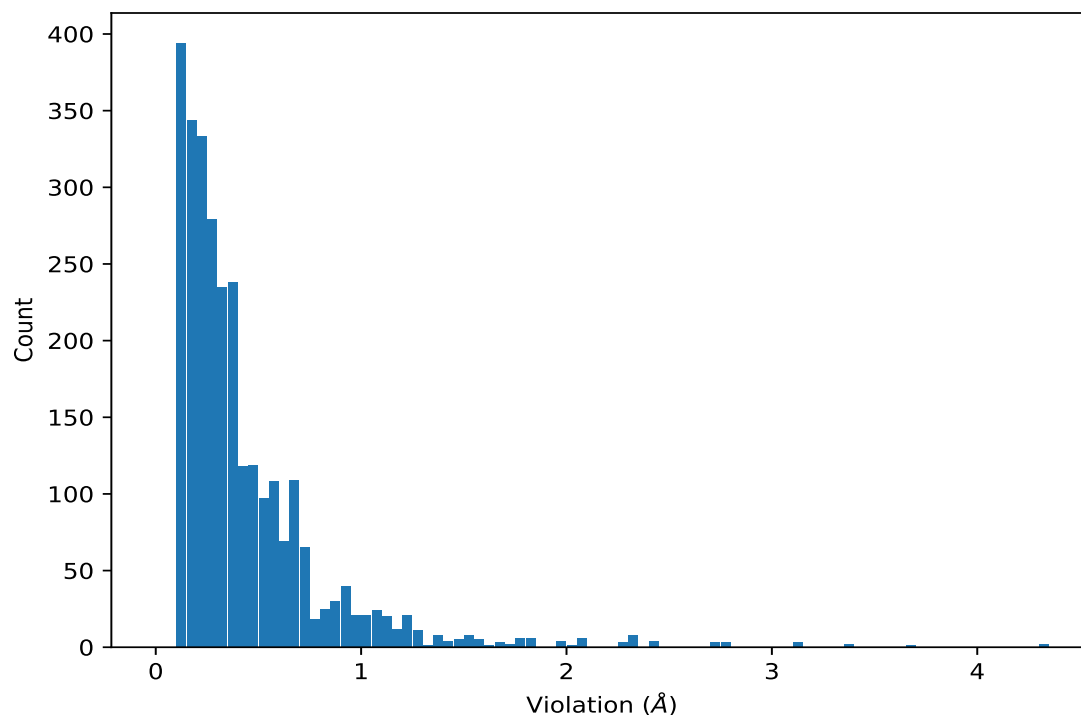
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1234)	1:14:A:GLU:H	1:17:A:ALA:HB2	2	0.12	0.0	0.12
(1,1234)	1:14:A:GLU:H	1:17:A:ALA:HB3	2	0.12	0.0	0.12
(1,1902)	1:59:A:ILE:HG21	1:61:A:LYS:HG2	2	0.12	0.0	0.12
(1,1902)	1:59:A:ILE:HG21	1:61:A:LYS:HG3	2	0.12	0.0	0.12
(1,1902)	1:59:A:ILE:HG22	1:61:A:LYS:HG2	2	0.12	0.0	0.12
(1,1902)	1:59:A:ILE:HG22	1:61:A:LYS:HG3	2	0.12	0.0	0.12
(1,1902)	1:59:A:ILE:HG23	1:61:A:LYS:HG2	2	0.12	0.0	0.12
(1,1902)	1:59:A:ILE:HG23	1:61:A:LYS:HG3	2	0.12	0.0	0.12
(1,553)	1:51:A:TRP:HB2	1:52:A:PHE:HD1	2	0.11	0.0	0.11
(1,553)	1:51:A:TRP:HB2	1:52:A:PHE:HD2	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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)
(1,1856)	1:51:A:TRP:HD1	1:54:A:ASN:HD21	3	4.34
(1,1856)	1:51:A:TRP:HD1	1:54:A:ASN:HD22	3	4.34
(1,1391)	1:51:A:TRP:HA	1:54:A:ASN:HD22	3	3.68
(1,1855)	1:51:A:TRP:HB2	1:54:A:ASN:HD21	3	3.39
(1,1855)	1:51:A:TRP:HB2	1:54:A:ASN:HD22	3	3.39
(1,1854)	1:51:A:TRP:HA	1:54:A:ASN:HD21	3	3.1
(1,1854)	1:51:A:TRP:HA	1:54:A:ASN:HD22	3	3.1
(1,732)	1:51:A:TRP:HA	1:54:A:ASN:HD21	3	3.1
(1,572)	1:50:A:ILE:HG21	1:54:A:ASN:HD22	3	2.76
(1,572)	1:50:A:ILE:HG22	1:54:A:ASN:HD22	3	2.76
(1,572)	1:50:A:ILE:HG23	1:54:A:ASN:HD22	3	2.76
(1,1387)	1:54:A:ASN:HD22	1:55:A:GLU:HA	1	2.73
(1,519)	1:44:A:ASN:HD21	1:46:A:ALA:HA	3	2.73
(1,519)	1:44:A:ASN:HD21	1:46:A:ALA:HA	2	2.71
(1,1219)	1:11:A:PHE:HD1	1:41:A:LEU:HG	1	2.44
(1,1219)	1:11:A:PHE:HD2	1:41:A:LEU:HG	1	2.44
(1,1219)	1:11:A:PHE:HD1	1:41:A:LEU:HG	3	2.4
(1,1219)	1:11:A:PHE:HD2	1:41:A:LEU:HG	3	2.4
(1,1852)	1:50:A:ILE:HD11	1:54:A:ASN:HD21	3	2.32
(1,1852)	1:50:A:ILE:HD11	1:54:A:ASN:HD22	3	2.32
(1,1852)	1:50:A:ILE:HD12	1:54:A:ASN:HD21	3	2.32
(1,1852)	1:50:A:ILE:HD12	1:54:A:ASN:HD22	3	2.32
(1,1852)	1:50:A:ILE:HD13	1:54:A:ASN:HD21	3	2.32
(1,1852)	1:50:A:ILE:HD13	1:54:A:ASN:HD22	3	2.32
(1,1219)	1:11:A:PHE:HD1	1:41:A:LEU:HG	2	2.31
(1,1219)	1:11:A:PHE:HD2	1:41:A:LEU:HG	2	2.31
(1,1856)	1:51:A:TRP:HD1	1:54:A:ASN:HD21	1	2.28
(1,1856)	1:51:A:TRP:HD1	1:54:A:ASN:HD22	1	2.28
(1,519)	1:44:A:ASN:HD21	1:46:A:ALA:HA	1	2.25
(1,1850)	1:50:A:ILE:HG21	1:54:A:ASN:HD21	3	2.08
(1,1850)	1:50:A:ILE:HG21	1:54:A:ASN:HD22	3	2.08
(1,1850)	1:50:A:ILE:HG22	1:54:A:ASN:HD21	3	2.08
(1,1850)	1:50:A:ILE:HG22	1:54:A:ASN:HD22	3	2.08
(1,1850)	1:50:A:ILE:HG23	1:54:A:ASN:HD21	3	2.08
(1,1850)	1:50:A:ILE:HG23	1:54:A:ASN:HD22	3	2.08
(1,1209)	1:29:A:LEU:HB3	1:49:A:LYS:HA	2	2.02
(1,1877)	1:54:A:ASN:HD21	1:55:A:GLU:HA	1	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1877)	1:54:A:ASN:HD22	1:55:A:GLU:HA	1	1.98
(1,1864)	1:53:A:GLN:H	1:54:A:ASN:HD21	3	1.97
(1,1864)	1:53:A:GLN:H	1:54:A:ASN:HD22	3	1.97
(1,1508)	1:9:A:THR:HG21	1:58:A:LYS:HG2	3	1.84
(1,1508)	1:9:A:THR:HG21	1:58:A:LYS:HG3	3	1.84
(1,1508)	1:9:A:THR:HG22	1:58:A:LYS:HG2	3	1.84
(1,1508)	1:9:A:THR:HG22	1:58:A:LYS:HG3	3	1.84
(1,1508)	1:9:A:THR:HG23	1:58:A:LYS:HG2	3	1.84
(1,1508)	1:9:A:THR:HG23	1:58:A:LYS:HG3	3	1.84
(1,1209)	1:29:A:LEU:HB3	1:49:A:LYS:HA	3	1.79
(1,1149)	1:50:A:ILE:HG21	1:54:A:ASN:HD21	3	1.79
(1,1149)	1:50:A:ILE:HG22	1:54:A:ASN:HD21	3	1.79
(1,1149)	1:50:A:ILE:HG23	1:54:A:ASN:HD21	3	1.79
(1,990)	1:29:A:LEU:HG	1:33:A:ARG:HB2	2	1.77
(1,990)	1:29:A:LEU:HG	1:33:A:ARG:HB3	2	1.77
(1,292)	1:12:A:SER:H	1:16:A:LEU:HB3	3	1.73
(1,64)	1:18:A:ARG:H	1:41:A:LEU:HG	2	1.7
(1,1391)	1:51:A:TRP:HA	1:54:A:ASN:HD22	1	1.69
(1,990)	1:29:A:LEU:HG	1:33:A:ARG:HB2	1	1.65
(1,990)	1:29:A:LEU:HG	1:33:A:ARG:HB3	1	1.65
(1,819)	1:54:A:ASN:HD21	1:55:A:GLU:HA	1	1.61
(1,1409)	1:34:A:ARG:HG2	1:45:A:GLU:HG2	3	1.59
(1,1409)	1:34:A:ARG:HG3	1:45:A:GLU:HG2	3	1.59
(1,1209)	1:29:A:LEU:HB3	1:49:A:LYS:HA	1	1.57
(1,1216)	1:15:A:GLN:HE21	1:43:A:LEU:HB2	2	1.56
(1,1216)	1:15:A:GLN:HE21	1:43:A:LEU:HB3	2	1.56
(1,1508)	1:9:A:THR:HG21	1:58:A:LYS:HG2	1	1.51
(1,1508)	1:9:A:THR:HG21	1:58:A:LYS:HG3	1	1.51
(1,1508)	1:9:A:THR:HG22	1:58:A:LYS:HG2	1	1.51
(1,1508)	1:9:A:THR:HG22	1:58:A:LYS:HG3	1	1.51
(1,1508)	1:9:A:THR:HG23	1:58:A:LYS:HG2	1	1.51
(1,1508)	1:9:A:THR:HG23	1:58:A:LYS:HG3	1	1.51
(1,990)	1:29:A:LEU:HG	1:33:A:ARG:HB2	3	1.51
(1,990)	1:29:A:LEU:HG	1:33:A:ARG:HB3	3	1.51
(1,1576)	1:15:A:GLN:HG2	1:41:A:LEU:HG	3	1.48
(1,1576)	1:15:A:GLN:HG3	1:41:A:LEU:HG	3	1.48
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD21	3	1.45
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD22	3	1.45
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD23	3	1.45
(1,1576)	1:15:A:GLN:HG2	1:41:A:LEU:HG	1	1.43
(1,1576)	1:15:A:GLN:HG3	1:41:A:LEU:HG	1	1.43
(1,690)	1:11:A:PHE:HZ	1:49:A:LYS:H	2	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1469)	1:15:A:GLN:HE21	1:43:A:LEU:H	2	1.4
(1,1576)	1:15:A:GLN:HG2	1:41:A:LEU:HG	2	1.39
(1,1576)	1:15:A:GLN:HG3	1:41:A:LEU:HG	2	1.39
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD21	3	1.35
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD22	3	1.35
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD23	3	1.35
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD21	3	1.35
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD22	3	1.35
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD23	3	1.35
(1,1284)	1:33:A:ARG:HD3	1:36:A:GLN:HB2	3	1.34
(1,1185)	1:50:A:ILE:HG21	1:53:A:GLN:HE21	3	1.29
(1,1185)	1:50:A:ILE:HG22	1:53:A:GLN:HE21	3	1.29
(1,1185)	1:50:A:ILE:HG23	1:53:A:GLN:HE21	3	1.29
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD21	2	1.29
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD22	2	1.29
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD23	2	1.29
(1,292)	1:12:A:SER:H	1:16:A:LEU:HB3	1	1.29
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD11	1	1.25
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD12	1	1.25
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD13	1	1.25
(1,542)	1:44:A:ASN:HD21	1:47:A:GLN:HG2	3	1.25
(1,1508)	1:9:A:THR:HG21	1:58:A:LYS:HG2	2	1.24
(1,1508)	1:9:A:THR:HG21	1:58:A:LYS:HG3	2	1.24
(1,1508)	1:9:A:THR:HG22	1:58:A:LYS:HG2	2	1.24
(1,1508)	1:9:A:THR:HG22	1:58:A:LYS:HG3	2	1.24
(1,1508)	1:9:A:THR:HG23	1:58:A:LYS:HG2	2	1.24
(1,1508)	1:9:A:THR:HG23	1:58:A:LYS:HG3	2	1.24
(1,1630)	1:20:A:LYS:HG2	1:24:A:ASN:HD21	3	1.23
(1,1630)	1:20:A:LYS:HG2	1:24:A:ASN:HD22	3	1.23
(1,1630)	1:20:A:LYS:HG3	1:24:A:ASN:HD21	3	1.23
(1,1630)	1:20:A:LYS:HG3	1:24:A:ASN:HD22	3	1.23
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD11	1	1.22
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD12	1	1.22
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD13	1	1.22
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD21	1	1.22
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD22	1	1.22
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD23	1	1.22
(1,1216)	1:15:A:GLN:HE21	1:43:A:LEU:HB2	1	1.21
(1,1216)	1:15:A:GLN:HE21	1:43:A:LEU:HB3	1	1.21
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD11	2	1.2
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD12	2	1.2
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD13	2	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1884)	1:56:A:ARG:H	1:58:A:LYS:HG2	1	1.19
(1,1884)	1:56:A:ARG:H	1:58:A:LYS:HG3	1	1.19
(1,1409)	1:34:A:ARG:HG2	1:45:A:GLU:HG2	2	1.19
(1,1409)	1:34:A:ARG:HG3	1:45:A:GLU:HG2	2	1.19
(1,1302)	1:18:A:ARG:HB2	1:41:A:LEU:H	1	1.19
(1,1302)	1:18:A:ARG:HB3	1:41:A:LEU:H	1	1.19
(1,690)	1:11:A:PHE:HZ	1:49:A:LYS:H	3	1.19
(1,1177)	1:19:A:LEU:HG	1:37:A:LEU:HB2	2	1.18
(1,805)	1:34:A:ARG:HD2	1:48:A:ILE:HA	2	1.15
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD11	3	1.15
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD12	3	1.15
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD13	3	1.15
(1,1325)	1:28:A:TYR:HA	1:53:A:GLN:HG3	2	1.14
(1,819)	1:54:A:ASN:HD21	1:55:A:GLU:HA	2	1.13
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD11	3	1.12
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD12	3	1.12
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD13	3	1.12
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD21	3	1.12
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD22	3	1.12
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD23	3	1.12
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD21	1	1.11
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD22	1	1.11
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD23	1	1.11
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD21	1	1.11
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD22	1	1.11
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD23	1	1.11
(1,813)	1:15:A:GLN:HA	1:41:A:LEU:HA	1	1.11
(1,64)	1:18:A:ARG:H	1:41:A:LEU:HG	1	1.11
(1,850)	1:34:A:ARG:HE	1:49:A:LYS:HA	2	1.1
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD11	1	1.1
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD12	1	1.1
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD13	1	1.1
(1,1574)	1:15:A:GLN:HG2	1:41:A:LEU:H	1	1.09
(1,1574)	1:15:A:GLN:HG3	1:41:A:LEU:H	1	1.09
(1,1185)	1:50:A:ILE:HG21	1:53:A:GLN:HE21	2	1.09
(1,1185)	1:50:A:ILE:HG22	1:53:A:GLN:HE21	2	1.09
(1,1185)	1:50:A:ILE:HG23	1:53:A:GLN:HE21	2	1.09
(1,1136)	1:38:A:SER:HB3	1:48:A:ILE:HG12	3	1.09
(1,1136)	1:38:A:SER:HB3	1:48:A:ILE:HG13	3	1.09
(1,690)	1:11:A:PHE:HZ	1:49:A:LYS:H	1	1.09
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD11	1	1.08
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD12	1	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD13	1	1.08
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD21	1	1.08
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD22	1	1.08
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD23	1	1.08
(1,805)	1:34:A:ARG:HD2	1:48:A:ILE:HA	1	1.08
(1,1386)	1:15:A:GLN:HA	1:41:A:LEU:HG	3	1.06
(1,1360)	1:51:A:TRP:HE3	1:55:A:GLU:HG3	2	1.05
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD21	3	1.05
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD22	3	1.05
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD23	3	1.05
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD11	3	1.05
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD12	3	1.05
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD13	3	1.05
(1,263)	1:15:A:GLN:HE21	1:42:A:GLY:H	1	1.05
(1,1325)	1:28:A:TYR:HA	1:53:A:GLN:HG3	3	1.04
(1,1190)	1:19:A:LEU:HD11	1:41:A:LEU:HG	2	1.04
(1,1190)	1:19:A:LEU:HD12	1:41:A:LEU:HG	2	1.04
(1,1190)	1:19:A:LEU:HD13	1:41:A:LEU:HG	2	1.04
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD11	1	1.04
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD12	1	1.04
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD13	1	1.04
(1,1386)	1:15:A:GLN:HA	1:41:A:LEU:HG	1	1.03
(1,1386)	1:15:A:GLN:HA	1:41:A:LEU:HG	2	1.03
(1,775)	1:55:A:GLU:HA	1:58:A:LYS:HG2	1	1.03
(1,282)	1:16:A:LEU:HA	1:20:A:LYS:HD2	2	1.03
(1,282)	1:16:A:LEU:HA	1:20:A:LYS:HD3	2	1.03
(1,64)	1:18:A:ARG:H	1:41:A:LEU:HG	3	1.03
(1,1190)	1:19:A:LEU:HD11	1:41:A:LEU:HG	3	1.02
(1,1190)	1:19:A:LEU:HD12	1:41:A:LEU:HG	3	1.02
(1,1190)	1:19:A:LEU:HD13	1:41:A:LEU:HG	3	1.02
(1,1469)	1:15:A:GLN:HE21	1:43:A:LEU:H	1	1.01
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD21	2	1.01
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD22	2	1.01
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD23	2	1.01
(1,408)	1:18:A:ARG:HE	1:19:A:LEU:H	2	1.01
(1,1409)	1:34:A:ARG:HG2	1:45:A:GLU:HG2	1	0.99
(1,1409)	1:34:A:ARG:HG3	1:45:A:GLU:HG2	1	0.99
(1,805)	1:34:A:ARG:HD2	1:48:A:ILE:HA	3	0.99
(1,610)	1:20:A:LYS:HG2	1:23:A:PHE:HD1	3	0.99
(1,610)	1:20:A:LYS:HG2	1:23:A:PHE:HD2	3	0.99
(1,610)	1:20:A:LYS:HG3	1:23:A:PHE:HD1	3	0.99
(1,610)	1:20:A:LYS:HG3	1:23:A:PHE:HD2	3	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1460)	1:19:A:LEU:HA	1:41:A:LEU:HG	2	0.98
(1,1460)	1:19:A:LEU:HA	1:41:A:LEU:HG	3	0.98
(1,727)	1:23:A:PHE:HZ	1:27:A:ARG:HD2	1	0.98
(1,1148)	1:51:A:TRP:HH2	1:59:A:ILE:HD11	3	0.97
(1,1148)	1:51:A:TRP:HH2	1:59:A:ILE:HD12	3	0.97
(1,1148)	1:51:A:TRP:HH2	1:59:A:ILE:HD13	3	0.97
(1,1216)	1:15:A:GLN:HE21	1:43:A:LEU:HB2	3	0.96
(1,1216)	1:15:A:GLN:HE21	1:43:A:LEU:HB3	3	0.96
(1,1190)	1:19:A:LEU:HD11	1:41:A:LEU:HG	1	0.96
(1,1190)	1:19:A:LEU:HD12	1:41:A:LEU:HG	1	0.96
(1,1190)	1:19:A:LEU:HD13	1:41:A:LEU:HG	1	0.96
(1,408)	1:18:A:ARG:HE	1:19:A:LEU:H	1	0.96
(1,1362)	1:21:A:ARG:H	1:21:A:ARG:HE	3	0.95
(1,321)	1:44:A:ASN:HD21	1:45:A:GLU:H	2	0.95
(1,1877)	1:54:A:ASN:HD21	1:55:A:GLU:HA	2	0.94
(1,1877)	1:54:A:ASN:HD22	1:55:A:GLU:HA	2	0.94
(1,807)	1:34:A:ARG:HD3	1:48:A:ILE:HA	2	0.94
(1,737)	1:9:A:THR:HA	1:51:A:TRP:HD1	3	0.94
(1,1884)	1:56:A:ARG:H	1:58:A:LYS:HG2	3	0.93
(1,1884)	1:56:A:ARG:H	1:58:A:LYS:HG3	3	0.93
(1,1574)	1:15:A:GLN:HG2	1:41:A:LEU:H	2	0.93
(1,1574)	1:15:A:GLN:HG3	1:41:A:LEU:H	2	0.93
(1,1136)	1:38:A:SER:HB3	1:48:A:ILE:HG12	2	0.93
(1,1136)	1:38:A:SER:HB3	1:48:A:ILE:HG13	2	0.93
(1,737)	1:9:A:THR:HA	1:51:A:TRP:HD1	2	0.93
(1,408)	1:18:A:ARG:HE	1:19:A:LEU:H	3	0.93
(1,292)	1:12:A:SER:H	1:16:A:LEU:HB3	2	0.93
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD11	1	0.92
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD12	1	0.92
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD13	1	0.92
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD21	1	0.92
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD22	1	0.92
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD23	1	0.92
(1,1628)	1:20:A:LYS:HA	1:24:A:ASN:HD21	3	0.92
(1,1628)	1:20:A:LYS:HA	1:24:A:ASN:HD22	3	0.92
(1,1136)	1:38:A:SER:HB3	1:48:A:ILE:HG12	1	0.92
(1,1136)	1:38:A:SER:HB3	1:48:A:ILE:HG13	1	0.92
(1,1460)	1:19:A:LEU:HA	1:41:A:LEU:HG	1	0.91
(1,1397)	1:19:A:LEU:HD11	1:48:A:ILE:H	1	0.91
(1,1397)	1:19:A:LEU:HD12	1:48:A:ILE:H	1	0.91
(1,1397)	1:19:A:LEU:HD13	1:48:A:ILE:H	1	0.91
(1,1360)	1:51:A:TRP:HE3	1:55:A:GLU:HG3	1	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1173)	1:19:A:LEU:HD21	1:37:A:LEU:HG	1	0.91
(1,1173)	1:19:A:LEU:HD22	1:37:A:LEU:HG	1	0.91
(1,1173)	1:19:A:LEU:HD23	1:37:A:LEU:HG	1	0.91
(1,931)	1:27:A:ARG:HB2	1:56:A:ARG:HD3	1	0.91
(1,1328)	1:28:A:TYR:HE1	1:53:A:GLN:HG3	2	0.9
(1,1328)	1:28:A:TYR:HE2	1:53:A:GLN:HG3	2	0.9
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD21	1	0.9
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD22	1	0.9
(1,1124)	1:33:A:ARG:HD3	1:37:A:LEU:HD23	1	0.9
(1,1056)	1:43:A:LEU:HD11	1:47:A:GLN:HE22	2	0.9
(1,1056)	1:43:A:LEU:HD12	1:47:A:GLN:HE22	2	0.9
(1,1056)	1:43:A:LEU:HD13	1:47:A:GLN:HE22	2	0.9
(1,1302)	1:18:A:ARG:HB2	1:41:A:LEU:H	2	0.89
(1,1302)	1:18:A:ARG:HB3	1:41:A:LEU:H	2	0.89
(1,716)	1:50:A:ILE:HD11	1:53:A:GLN:HE21	2	0.88
(1,716)	1:50:A:ILE:HD12	1:53:A:GLN:HE21	2	0.88
(1,716)	1:50:A:ILE:HD13	1:53:A:GLN:HE21	2	0.88
(1,1910)	1:61:A:LYS:H	1:61:A:LYS:HD2	3	0.87
(1,1910)	1:61:A:LYS:H	1:61:A:LYS:HD3	3	0.87
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD11	3	0.87
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD12	3	0.87
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD13	3	0.87
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD21	3	0.87
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD22	3	0.87
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD23	3	0.87
(1,1286)	1:19:A:LEU:HA	1:20:A:LYS:HD2	2	0.87
(1,1286)	1:19:A:LEU:HA	1:20:A:LYS:HD3	2	0.87
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD21	1	0.87
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD22	1	0.87
(1,1016)	1:41:A:LEU:H	1:43:A:LEU:HD23	1	0.87
(1,610)	1:20:A:LYS:HG2	1:23:A:PHE:HD1	2	0.87
(1,610)	1:20:A:LYS:HG2	1:23:A:PHE:HD2	2	0.87
(1,610)	1:20:A:LYS:HG3	1:23:A:PHE:HD1	2	0.87
(1,610)	1:20:A:LYS:HG3	1:23:A:PHE:HD2	2	0.87
(1,297)	1:11:A:PHE:HE1	1:12:A:SER:H	3	0.87
(1,297)	1:11:A:PHE:HE2	1:12:A:SER:H	3	0.87
(1,1325)	1:28:A:TYR:HA	1:53:A:GLN:HG3	1	0.86
(1,282)	1:16:A:LEU:HA	1:20:A:LYS:HD2	1	0.86
(1,282)	1:16:A:LEU:HA	1:20:A:LYS:HD3	1	0.86
(1,282)	1:16:A:LEU:HA	1:20:A:LYS:HD2	3	0.86
(1,282)	1:16:A:LEU:HA	1:20:A:LYS:HD3	3	0.86
(1,790)	1:51:A:TRP:HA	1:55:A:GLU:HA	1	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1469)	1:15:A:GLN:HE21	1:43:A:LEU:H	3	0.84
(1,1360)	1:51:A:TRP:HE3	1:55:A:GLU:HG3	3	0.84
(1,1286)	1:19:A:LEU:HA	1:20:A:LYS:HD2	1	0.84
(1,1286)	1:19:A:LEU:HA	1:20:A:LYS:HD3	1	0.84
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD21	3	0.84
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD22	3	0.84
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD23	3	0.84
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD11	2	0.84
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD12	2	0.84
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD13	2	0.84
(1,312)	1:43:A:LEU:HG	1:44:A:ASN:H	3	0.84
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD11	2	0.83
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD12	2	0.83
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD13	2	0.83
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD21	2	0.83
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD22	2	0.83
(1,1809)	1:41:A:LEU:H	1:43:A:LEU:HD23	2	0.83
(1,341)	1:12:A:SER:HB3	1:14:A:GLU:H	2	0.82
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD11	3	0.81
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD12	3	0.81
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD13	3	0.81
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD21	3	0.81
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD22	3	0.81
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD23	3	0.81
(1,770)	1:52:A:PHE:HA	1:55:A:GLU:HG3	2	0.8
(1,1012)	1:30:A:THR:HG21	1:32:A:ARG:H	1	0.78
(1,1012)	1:30:A:THR:HG22	1:32:A:ARG:H	1	0.78
(1,1012)	1:30:A:THR:HG23	1:32:A:ARG:H	1	0.78
(1,716)	1:50:A:ILE:HD11	1:53:A:GLN:HE21	3	0.78
(1,716)	1:50:A:ILE:HD12	1:53:A:GLN:HE21	3	0.78
(1,716)	1:50:A:ILE:HD13	1:53:A:GLN:HE21	3	0.78
(1,1107)	1:29:A:LEU:HG	1:34:A:ARG:H	1	0.77
(1,1107)	1:29:A:LEU:HG	1:34:A:ARG:H	3	0.77
(1,1740)	1:30:A:THR:HA	1:31:A:GLU:HG2	3	0.76
(1,1740)	1:30:A:THR:HA	1:31:A:GLU:HG3	3	0.76
(1,1116)	1:59:A:ILE:HG21	1:61:A:LYS:HG3	2	0.76
(1,1116)	1:59:A:ILE:HG22	1:61:A:LYS:HG3	2	0.76
(1,1116)	1:59:A:ILE:HG23	1:61:A:LYS:HG3	2	0.76
(1,798)	1:45:A:GLU:HA	1:49:A:LYS:HA	3	0.76
(1,1177)	1:19:A:LEU:HG	1:37:A:LEU:HB2	3	0.75
(1,1107)	1:29:A:LEU:HG	1:34:A:ARG:H	2	0.75
(1,931)	1:27:A:ARG:HB2	1:56:A:ARG:HD3	3	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,807)	1:34:A:ARG:HD3	1:48:A:ILE:HA	1	0.75
(1,1824)	1:43:A:LEU:HD11	1:45:A:GLU:HA	1	0.74
(1,1824)	1:43:A:LEU:HD12	1:45:A:GLU:HA	1	0.74
(1,1824)	1:43:A:LEU:HD13	1:45:A:GLU:HA	1	0.74
(1,1824)	1:43:A:LEU:HD21	1:45:A:GLU:HA	1	0.74
(1,1824)	1:43:A:LEU:HD22	1:45:A:GLU:HA	1	0.74
(1,1824)	1:43:A:LEU:HD23	1:45:A:GLU:HA	1	0.74
(1,1817)	1:41:A:LEU:HD11	1:43:A:LEU:H	2	0.74
(1,1817)	1:41:A:LEU:HD12	1:43:A:LEU:H	2	0.74
(1,1817)	1:41:A:LEU:HD13	1:43:A:LEU:H	2	0.74
(1,1817)	1:41:A:LEU:HD21	1:43:A:LEU:H	2	0.74
(1,1817)	1:41:A:LEU:HD22	1:43:A:LEU:H	2	0.74
(1,1817)	1:41:A:LEU:HD23	1:43:A:LEU:H	2	0.74
(1,1609)	1:18:A:ARG:HD2	1:22:A:GLU:H	1	0.74
(1,1609)	1:18:A:ARG:HD3	1:22:A:GLU:H	1	0.74
(1,1177)	1:19:A:LEU:HG	1:37:A:LEU:HB2	1	0.74
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD21	1	0.74
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD22	1	0.74
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD23	1	0.74
(1,850)	1:34:A:ARG:HE	1:49:A:LYS:HA	1	0.74
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD11	3	0.73
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD12	3	0.73
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD13	3	0.73
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD21	3	0.73
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD22	3	0.73
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD23	3	0.73
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD11	3	0.73
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD12	3	0.73
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD13	3	0.73
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD21	3	0.73
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD22	3	0.73
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD23	3	0.73
(1,1302)	1:18:A:ARG:HB2	1:41:A:LEU:H	3	0.73
(1,1302)	1:18:A:ARG:HB3	1:41:A:LEU:H	3	0.73
(1,1148)	1:51:A:TRP:HH2	1:59:A:ILE:HD11	1	0.73
(1,1148)	1:51:A:TRP:HH2	1:59:A:ILE:HD12	1	0.73
(1,1148)	1:51:A:TRP:HH2	1:59:A:ILE:HD13	1	0.73
(1,833)	1:30:A:THR:H	1:33:A:ARG:HD2	1	0.73
(1,727)	1:23:A:PHE:HZ	1:27:A:ARG:HD2	3	0.73
(1,1397)	1:19:A:LEU:HD11	1:48:A:ILE:H	2	0.72
(1,1397)	1:19:A:LEU:HD12	1:48:A:ILE:H	2	0.72
(1,1397)	1:19:A:LEU:HD13	1:48:A:ILE:H	2	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,880)	1:22:A:GLU:HG2	1:37:A:LEU:HA	2	0.72
(1,880)	1:22:A:GLU:HG3	1:37:A:LEU:HA	2	0.72
(1,1870)	1:54:A:ASN:H	1:54:A:ASN:HD21	3	0.71
(1,1870)	1:54:A:ASN:H	1:54:A:ASN:HD22	3	0.71
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD21	2	0.71
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD22	2	0.71
(1,1359)	1:11:A:PHE:HD1	1:41:A:LEU:HD23	2	0.71
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD21	2	0.71
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD22	2	0.71
(1,1359)	1:11:A:PHE:HD2	1:41:A:LEU:HD23	2	0.71
(1,1116)	1:59:A:ILE:HG21	1:61:A:LYS:HG3	3	0.71
(1,1116)	1:59:A:ILE:HG22	1:61:A:LYS:HG3	3	0.71
(1,1116)	1:59:A:ILE:HG23	1:61:A:LYS:HG3	3	0.71
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD21	2	0.71
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD22	2	0.71
(1,1095)	1:38:A:SER:HA	1:43:A:LEU:HD23	2	0.71
(1,869)	1:58:A:LYS:HA	1:58:A:LYS:HE3	1	0.71
(1,1389)	1:35:A:GLN:HE21	1:36:A:GLN:HG2	3	0.7
(1,1389)	1:35:A:GLN:HE21	1:36:A:GLN:HG3	3	0.7
(1,1057)	1:19:A:LEU:HD21	1:48:A:ILE:H	1	0.7
(1,1057)	1:19:A:LEU:HD22	1:48:A:ILE:H	1	0.7
(1,1057)	1:19:A:LEU:HD23	1:48:A:ILE:H	1	0.7
(1,869)	1:58:A:LYS:HA	1:58:A:LYS:HE3	3	0.7
(1,807)	1:34:A:ARG:HD3	1:48:A:ILE:HA	3	0.7
(1,1817)	1:41:A:LEU:HD11	1:43:A:LEU:H	3	0.69
(1,1817)	1:41:A:LEU:HD12	1:43:A:LEU:H	3	0.69
(1,1817)	1:41:A:LEU:HD13	1:43:A:LEU:H	3	0.69
(1,1817)	1:41:A:LEU:HD21	1:43:A:LEU:H	3	0.69
(1,1817)	1:41:A:LEU:HD22	1:43:A:LEU:H	3	0.69
(1,1817)	1:41:A:LEU:HD23	1:43:A:LEU:H	3	0.69
(1,1738)	1:29:A:LEU:HD11	1:53:A:GLN:H	2	0.69
(1,1738)	1:29:A:LEU:HD12	1:53:A:GLN:H	2	0.69
(1,1738)	1:29:A:LEU:HD13	1:53:A:GLN:H	2	0.69
(1,1738)	1:29:A:LEU:HD21	1:53:A:GLN:H	2	0.69
(1,1738)	1:29:A:LEU:HD22	1:53:A:GLN:H	2	0.69
(1,1738)	1:29:A:LEU:HD23	1:53:A:GLN:H	2	0.69
(1,1461)	1:32:A:ARG:HA	1:35:A:GLN:HB3	1	0.69
(1,1173)	1:19:A:LEU:HD21	1:37:A:LEU:HG	2	0.69
(1,1173)	1:19:A:LEU:HD22	1:37:A:LEU:HG	2	0.69
(1,1173)	1:19:A:LEU:HD23	1:37:A:LEU:HG	2	0.69
(1,1131)	1:34:A:ARG:HA	1:48:A:ILE:HG12	1	0.69
(1,1131)	1:34:A:ARG:HA	1:48:A:ILE:HG13	1	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD11	3	0.69
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD12	3	0.69
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD13	3	0.69
(1,1910)	1:61:A:LYS:H	1:61:A:LYS:HD2	1	0.68
(1,1910)	1:61:A:LYS:H	1:61:A:LYS:HD3	1	0.68
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD11	1	0.68
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD12	1	0.68
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD13	1	0.68
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD21	1	0.68
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD22	1	0.68
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD23	1	0.68
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD11	1	0.68
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD12	1	0.68
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD13	1	0.68
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD21	1	0.68
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD22	1	0.68
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD23	1	0.68
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD11	1	0.68
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD12	1	0.68
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD13	1	0.68
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD21	1	0.68
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD22	1	0.68
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD23	1	0.68
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD11	1	0.68
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD12	1	0.68
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD13	1	0.68
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD21	1	0.68
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD22	1	0.68
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD23	1	0.68
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD11	1	0.68
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD12	1	0.68
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD13	1	0.68
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD21	1	0.68
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD22	1	0.68
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD23	1	0.68
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD11	1	0.68
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD12	1	0.68
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD13	1	0.68
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD21	1	0.68
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD22	1	0.68
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD23	1	0.68
(1,1712)	1:29:A:LEU:HD11	1:33:A:ARG:HD2	1	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1712)	1:29:A:LEU:HD11	1:33:A:ARG:HD3	1	0.68
(1,1712)	1:29:A:LEU:HD12	1:33:A:ARG:HD2	1	0.68
(1,1712)	1:29:A:LEU:HD12	1:33:A:ARG:HD3	1	0.68
(1,1712)	1:29:A:LEU:HD13	1:33:A:ARG:HD2	1	0.68
(1,1712)	1:29:A:LEU:HD13	1:33:A:ARG:HD3	1	0.68
(1,1712)	1:29:A:LEU:HD21	1:33:A:ARG:HD2	1	0.68
(1,1712)	1:29:A:LEU:HD21	1:33:A:ARG:HD3	1	0.68
(1,1712)	1:29:A:LEU:HD22	1:33:A:ARG:HD2	1	0.68
(1,1712)	1:29:A:LEU:HD22	1:33:A:ARG:HD3	1	0.68
(1,1712)	1:29:A:LEU:HD23	1:33:A:ARG:HD2	1	0.68
(1,1712)	1:29:A:LEU:HD23	1:33:A:ARG:HD3	1	0.68
(1,1373)	1:23:A:PHE:HE1	1:27:A:ARG:HD2	1	0.68
(1,1373)	1:23:A:PHE:HE2	1:27:A:ARG:HD2	1	0.68
(1,1367)	1:44:A:ASN:HD21	1:47:A:GLN:H	3	0.68
(1,1180)	1:38:A:SER:HA	1:43:A:LEU:HG	3	0.68
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG21	3	0.68
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG22	3	0.68
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG23	3	0.68
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD11	3	0.68
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD12	3	0.68
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD13	3	0.68
(1,903)	1:34:A:ARG:HD3	1:49:A:LYS:HD3	1	0.68
(1,1634)	1:21:A:ARG:HA	1:24:A:ASN:HB2	2	0.67
(1,1634)	1:21:A:ARG:HA	1:24:A:ASN:HB3	2	0.67
(1,850)	1:34:A:ARG:HE	1:49:A:LYS:HA	3	0.67
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD11	2	0.67
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD12	2	0.67
(1,534)	1:42:A:GLY:H	1:43:A:LEU:HD13	2	0.67
(1,151)	1:35:A:GLN:HE22	1:36:A:GLN:HB3	2	0.67
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD11	2	0.66
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD12	2	0.66
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD13	2	0.66
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD21	2	0.66
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD22	2	0.66
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD23	2	0.66
(1,1387)	1:54:A:ASN:HD22	1:55:A:GLU:HA	2	0.66
(1,1179)	1:43:A:LEU:HG	1:47:A:GLN:HB2	2	0.66
(1,1013)	1:41:A:LEU:H	1:43:A:LEU:HG	1	0.66
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD11	3	0.66
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD12	3	0.66
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD13	3	0.66
(1,321)	1:44:A:ASN:HD21	1:45:A:GLU:H	1	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1494)	1:6:A:ARG:HB2	1:7:A:PRO:HG2	1	0.65
(1,1494)	1:6:A:ARG:HB3	1:7:A:PRO:HG2	1	0.65
(1,1345)	1:20:A:LYS:HE2	1:51:A:TRP:HE1	1	0.65
(1,1345)	1:20:A:LYS:HE3	1:51:A:TRP:HE1	1	0.65
(1,833)	1:30:A:THR:H	1:33:A:ARG:HD2	3	0.65
(1,790)	1:51:A:TRP:HA	1:55:A:GLU:HA	3	0.65
(1,263)	1:15:A:GLN:HE21	1:42:A:GLY:H	3	0.65
(1,1847)	1:50:A:ILE:H	1:53:A:GLN:HE21	2	0.64
(1,1847)	1:50:A:ILE:H	1:53:A:GLN:HE22	2	0.64
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD11	1	0.64
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD12	1	0.64
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD13	1	0.64
(1,798)	1:45:A:GLU:HA	1:49:A:LYS:HA	2	0.64
(1,610)	1:20:A:LYS:HG2	1:23:A:PHE:HD1	1	0.64
(1,610)	1:20:A:LYS:HG2	1:23:A:PHE:HD2	1	0.64
(1,610)	1:20:A:LYS:HG3	1:23:A:PHE:HD1	1	0.64
(1,610)	1:20:A:LYS:HG3	1:23:A:PHE:HD2	1	0.64
(1,415)	1:5:A:LYS:HA	1:6:A:ARG:H	3	0.64
(1,263)	1:15:A:GLN:HE21	1:42:A:GLY:H	2	0.64
(1,1877)	1:54:A:ASN:HD21	1:55:A:GLU:HA	3	0.63
(1,1877)	1:54:A:ASN:HD22	1:55:A:GLU:HA	3	0.63
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD11	3	0.63
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD12	3	0.63
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD13	3	0.63
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD21	3	0.63
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD22	3	0.63
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD23	3	0.63
(1,1639)	1:21:A:ARG:HB2	1:22:A:GLU:HA	3	0.63
(1,1639)	1:21:A:ARG:HB3	1:22:A:GLU:HA	3	0.63
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD21	3	0.63
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD22	3	0.63
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD23	3	0.63
(1,903)	1:34:A:ARG:HD3	1:49:A:LYS:HD3	2	0.63
(1,1839)	1:49:A:LYS:HA	1:49:A:LYS:HD2	2	0.62
(1,1839)	1:49:A:LYS:HA	1:49:A:LYS:HD3	2	0.62
(1,1574)	1:15:A:GLN:HG2	1:41:A:LEU:H	3	0.62
(1,1574)	1:15:A:GLN:HG3	1:41:A:LEU:H	3	0.62
(1,1463)	1:11:A:PHE:HB3	1:15:A:GLN:H	2	0.62
(1,1131)	1:34:A:ARG:HA	1:48:A:ILE:HG12	2	0.62
(1,1131)	1:34:A:ARG:HA	1:48:A:ILE:HG13	2	0.62
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD11	3	0.62
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD12	3	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD13	3	0.62
(1,1062)	1:52:A:PHE:HB3	1:55:A:GLU:HB2	1	0.62
(1,905)	1:9:A:THR:HG21	1:51:A:TRP:HB2	3	0.62
(1,905)	1:9:A:THR:HG22	1:51:A:TRP:HB2	3	0.62
(1,905)	1:9:A:THR:HG23	1:51:A:TRP:HB2	3	0.62
(1,321)	1:44:A:ASN:HD21	1:45:A:GLU:H	3	0.62
(1,102)	1:29:A:LEU:HA	1:33:A:ARG:HE	2	0.62
(1,1366)	1:56:A:ARG:H	1:56:A:ARG:HE	2	0.61
(1,819)	1:54:A:ASN:HD21	1:55:A:GLU:HA	3	0.61
(1,727)	1:23:A:PHE:HZ	1:27:A:ARG:HD2	2	0.61
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD21	1	0.61
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD22	1	0.61
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD23	1	0.61
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD21	1	0.61
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD22	1	0.61
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD23	1	0.61
(1,542)	1:44:A:ASN:HD21	1:47:A:GLN:HG2	2	0.61
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD11	1	0.61
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD12	1	0.61
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD13	1	0.61
(1,151)	1:35:A:GLN:HE22	1:36:A:GLN:HB3	1	0.61
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD11	1	0.6
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD12	1	0.6
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD13	1	0.6
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD21	1	0.6
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD22	1	0.6
(1,1820)	1:42:A:GLY:H	1:43:A:LEU:HD23	1	0.6
(1,1364)	1:30:A:THR:H	1:33:A:ARG:HE	2	0.6
(1,1179)	1:43:A:LEU:HG	1:47:A:GLN:HB2	3	0.6
(1,1062)	1:52:A:PHE:HB3	1:55:A:GLU:HB2	3	0.6
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD11	2	0.6
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD12	2	0.6
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD13	2	0.6
(1,315)	1:44:A:ASN:H	1:47:A:GLN:HB3	3	0.6
(1,1839)	1:49:A:LYS:HA	1:49:A:LYS:HD2	1	0.59
(1,1839)	1:49:A:LYS:HA	1:49:A:LYS:HD3	1	0.59
(1,1817)	1:41:A:LEU:HD11	1:43:A:LEU:H	1	0.59
(1,1817)	1:41:A:LEU:HD12	1:43:A:LEU:H	1	0.59
(1,1817)	1:41:A:LEU:HD13	1:43:A:LEU:H	1	0.59
(1,1817)	1:41:A:LEU:HD21	1:43:A:LEU:H	1	0.59
(1,1817)	1:41:A:LEU:HD22	1:43:A:LEU:H	1	0.59
(1,1817)	1:41:A:LEU:HD23	1:43:A:LEU:H	1	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1470)	1:11:A:PHE:HE1	1:47:A:GLN:HE21	1	0.59
(1,1470)	1:11:A:PHE:HE2	1:47:A:GLN:HE21	1	0.59
(1,1365)	1:38:A:SER:H	1:42:A:GLY:H	3	0.59
(1,1364)	1:30:A:THR:H	1:33:A:ARG:HE	3	0.59
(1,1233)	1:30:A:THR:HG21	1:34:A:ARG:H	1	0.59
(1,1233)	1:30:A:THR:HG22	1:34:A:ARG:H	1	0.59
(1,1233)	1:30:A:THR:HG23	1:34:A:ARG:H	1	0.59
(1,1160)	1:38:A:SER:H	1:48:A:ILE:HG12	2	0.59
(1,1160)	1:38:A:SER:H	1:48:A:ILE:HG13	2	0.59
(1,798)	1:45:A:GLU:HA	1:49:A:LYS:HA	1	0.59
(1,559)	1:29:A:LEU:H	1:52:A:PHE:HD1	2	0.59
(1,559)	1:29:A:LEU:H	1:52:A:PHE:HD2	2	0.59
(1,526)	1:23:A:PHE:HZ	1:55:A:GLU:H	2	0.59
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD11	1	0.58
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD12	1	0.58
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD13	1	0.58
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD21	1	0.58
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD22	1	0.58
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD23	1	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD11	1	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD12	1	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD13	1	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD21	1	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD22	1	0.58
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD23	1	0.58
(1,1629)	1:20:A:LYS:HB2	1:24:A:ASN:HD21	3	0.58
(1,1629)	1:20:A:LYS:HB2	1:24:A:ASN:HD22	3	0.58
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD11	3	0.58
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD12	3	0.58
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD13	3	0.58
(1,1179)	1:43:A:LEU:HG	1:47:A:GLN:HB2	1	0.58
(1,695)	1:11:A:PHE:HZ	1:47:A:GLN:H	3	0.58
(1,312)	1:43:A:LEU:HG	1:44:A:ASN:H	2	0.58
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD11	3	0.57
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD12	3	0.57
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD13	3	0.57
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD21	3	0.57
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD22	3	0.57
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD23	3	0.57
(1,1669)	1:24:A:ASN:HD21	1:25:A:GLU:HA	1	0.57
(1,1669)	1:24:A:ASN:HD22	1:25:A:GLU:HA	1	0.57
(1,1482)	1:11:A:PHE:HB2	1:16:A:LEU:HB2	1	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1390)	1:21:A:ARG:HA	1:21:A:ARG:HE	3	0.57
(1,1110)	1:19:A:LEU:HD21	1:41:A:LEU:HD21	3	0.57
(1,1110)	1:19:A:LEU:HD21	1:41:A:LEU:HD22	3	0.57
(1,1110)	1:19:A:LEU:HD21	1:41:A:LEU:HD23	3	0.57
(1,1110)	1:19:A:LEU:HD22	1:41:A:LEU:HD21	3	0.57
(1,1110)	1:19:A:LEU:HD22	1:41:A:LEU:HD22	3	0.57
(1,1110)	1:19:A:LEU:HD22	1:41:A:LEU:HD23	3	0.57
(1,1110)	1:19:A:LEU:HD23	1:41:A:LEU:HD21	3	0.57
(1,1110)	1:19:A:LEU:HD23	1:41:A:LEU:HD22	3	0.57
(1,1110)	1:19:A:LEU:HD23	1:41:A:LEU:HD23	3	0.57
(1,1062)	1:52:A:PHE:HB3	1:55:A:GLU:HB2	2	0.57
(1,888)	1:53:A:GLN:HG2	1:54:A:ASN:HA	1	0.57
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD11	1	0.57
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD12	1	0.57
(1,873)	1:40:A:GLU:HA	1:41:A:LEU:HD13	1	0.57
(1,834)	1:30:A:THR:H	1:34:A:ARG:HD3	3	0.57
(1,832)	1:53:A:GLN:HA	1:53:A:GLN:HE22	2	0.57
(1,295)	1:13:A:SER:H	1:17:A:ALA:H	3	0.57
(1,269)	1:11:A:PHE:H	1:11:A:PHE:HE1	1	0.57
(1,269)	1:11:A:PHE:H	1:11:A:PHE:HE2	1	0.57
(1,1815)	1:41:A:LEU:HD11	1:42:A:GLY:H	1	0.56
(1,1815)	1:41:A:LEU:HD12	1:42:A:GLY:H	1	0.56
(1,1815)	1:41:A:LEU:HD13	1:42:A:GLY:H	1	0.56
(1,1815)	1:41:A:LEU:HD21	1:42:A:GLY:H	1	0.56
(1,1815)	1:41:A:LEU:HD22	1:42:A:GLY:H	1	0.56
(1,1815)	1:41:A:LEU:HD23	1:42:A:GLY:H	1	0.56
(1,1634)	1:21:A:ARG:HA	1:24:A:ASN:HB2	1	0.56
(1,1634)	1:21:A:ARG:HA	1:24:A:ASN:HB3	1	0.56
(1,1540)	1:12:A:SER:HB2	1:15:A:GLN:H	2	0.56
(1,1540)	1:12:A:SER:HB3	1:15:A:GLN:H	2	0.56
(1,1160)	1:38:A:SER:H	1:48:A:ILE:HG12	1	0.56
(1,1160)	1:38:A:SER:H	1:48:A:ILE:HG13	1	0.56
(1,346)	1:44:A:ASN:H	1:47:A:GLN:HA	3	0.56
(1,1910)	1:61:A:LYS:H	1:61:A:LYS:HD2	2	0.55
(1,1910)	1:61:A:LYS:H	1:61:A:LYS:HD3	2	0.55
(1,1824)	1:43:A:LEU:HD11	1:45:A:GLU:HA	2	0.55
(1,1824)	1:43:A:LEU:HD12	1:45:A:GLU:HA	2	0.55
(1,1824)	1:43:A:LEU:HD13	1:45:A:GLU:HA	2	0.55
(1,1824)	1:43:A:LEU:HD21	1:45:A:GLU:HA	2	0.55
(1,1824)	1:43:A:LEU:HD22	1:45:A:GLU:HA	2	0.55
(1,1824)	1:43:A:LEU:HD23	1:45:A:GLU:HA	2	0.55
(1,1748)	1:32:A:ARG:HA	1:32:A:ARG:HD2	1	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1748)	1:32:A:ARG:HA	1:32:A:ARG:HD3	1	0.55
(1,1585)	1:16:A:LEU:HD11	1:18:A:ARG:H	1	0.55
(1,1585)	1:16:A:LEU:HD12	1:18:A:ARG:H	1	0.55
(1,1585)	1:16:A:LEU:HD13	1:18:A:ARG:H	1	0.55
(1,1585)	1:16:A:LEU:HD21	1:18:A:ARG:H	1	0.55
(1,1585)	1:16:A:LEU:HD22	1:18:A:ARG:H	1	0.55
(1,1585)	1:16:A:LEU:HD23	1:18:A:ARG:H	1	0.55
(1,1245)	1:37:A:LEU:HB2	1:48:A:ILE:HG12	1	0.55
(1,1245)	1:37:A:LEU:HB2	1:48:A:ILE:HG13	1	0.55
(1,764)	1:24:A:ASN:H	1:51:A:TRP:HZ3	2	0.55
(1,764)	1:24:A:ASN:H	1:51:A:TRP:HZ3	3	0.55
(1,346)	1:44:A:ASN:H	1:47:A:GLN:HA	1	0.55
(1,312)	1:43:A:LEU:HG	1:44:A:ASN:H	1	0.55
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD11	2	0.55
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD12	2	0.55
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD13	2	0.55
(1,1824)	1:43:A:LEU:HD11	1:45:A:GLU:HA	3	0.54
(1,1824)	1:43:A:LEU:HD12	1:45:A:GLU:HA	3	0.54
(1,1824)	1:43:A:LEU:HD13	1:45:A:GLU:HA	3	0.54
(1,1824)	1:43:A:LEU:HD21	1:45:A:GLU:HA	3	0.54
(1,1824)	1:43:A:LEU:HD22	1:45:A:GLU:HA	3	0.54
(1,1824)	1:43:A:LEU:HD23	1:45:A:GLU:HA	3	0.54
(1,1343)	1:22:A:GLU:HG2	1:37:A:LEU:H	2	0.54
(1,1343)	1:22:A:GLU:HG3	1:37:A:LEU:H	2	0.54
(1,1064)	1:19:A:LEU:HD21	1:22:A:GLU:HB3	1	0.54
(1,1064)	1:19:A:LEU:HD22	1:22:A:GLU:HB3	1	0.54
(1,1064)	1:19:A:LEU:HD23	1:22:A:GLU:HB3	1	0.54
(1,1233)	1:30:A:THR:HG21	1:34:A:ARG:H	2	0.53
(1,1233)	1:30:A:THR:HG22	1:34:A:ARG:H	2	0.53
(1,1233)	1:30:A:THR:HG23	1:34:A:ARG:H	2	0.53
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG21	2	0.53
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG22	2	0.53
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG23	2	0.53
(1,1135)	1:37:A:LEU:HA	1:48:A:ILE:HG12	1	0.53
(1,1135)	1:37:A:LEU:HA	1:48:A:ILE:HG13	1	0.53
(1,833)	1:30:A:THR:H	1:33:A:ARG:HD2	2	0.53
(1,564)	1:47:A:GLN:HA	1:47:A:GLN:HE21	1	0.53
(1,34)	1:16:A:LEU:HD11	1:51:A:TRP:HH2	1	0.53
(1,34)	1:16:A:LEU:HD12	1:51:A:TRP:HH2	1	0.53
(1,34)	1:16:A:LEU:HD13	1:51:A:TRP:HH2	1	0.53
(1,1790)	1:37:A:LEU:HD11	1:51:A:TRP:HB3	1	0.52
(1,1790)	1:37:A:LEU:HD12	1:51:A:TRP:HB3	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1790)	1:37:A:LEU:HD13	1:51:A:TRP:HB3	1	0.52
(1,1790)	1:37:A:LEU:HD21	1:51:A:TRP:HB3	1	0.52
(1,1790)	1:37:A:LEU:HD22	1:51:A:TRP:HB3	1	0.52
(1,1790)	1:37:A:LEU:HD23	1:51:A:TRP:HB3	1	0.52
(1,1418)	1:11:A:PHE:HB2	1:16:A:LEU:HB3	1	0.52
(1,1404)	1:34:A:ARG:HD3	1:45:A:GLU:HA	3	0.52
(1,1057)	1:19:A:LEU:HD21	1:48:A:ILE:H	2	0.52
(1,1057)	1:19:A:LEU:HD22	1:48:A:ILE:H	2	0.52
(1,1057)	1:19:A:LEU:HD23	1:48:A:ILE:H	2	0.52
(1,1047)	1:29:A:LEU:HD21	1:52:A:PHE:HB2	2	0.52
(1,1047)	1:29:A:LEU:HD22	1:52:A:PHE:HB2	2	0.52
(1,1047)	1:29:A:LEU:HD23	1:52:A:PHE:HB2	2	0.52
(1,898)	1:21:A:ARG:HD2	1:22:A:GLU:H	3	0.52
(1,898)	1:21:A:ARG:HD3	1:22:A:GLU:H	3	0.52
(1,770)	1:52:A:PHE:HA	1:55:A:GLU:HG3	1	0.52
(1,364)	1:48:A:ILE:HB	1:52:A:PHE:H	3	0.52
(1,1903)	1:59:A:ILE:HG21	1:61:A:LYS:HD2	3	0.51
(1,1903)	1:59:A:ILE:HG21	1:61:A:LYS:HD3	3	0.51
(1,1903)	1:59:A:ILE:HG22	1:61:A:LYS:HD2	3	0.51
(1,1903)	1:59:A:ILE:HG22	1:61:A:LYS:HD3	3	0.51
(1,1903)	1:59:A:ILE:HG23	1:61:A:LYS:HD2	3	0.51
(1,1903)	1:59:A:ILE:HG23	1:61:A:LYS:HD3	3	0.51
(1,1828)	1:43:A:LEU:HD11	1:48:A:ILE:H	2	0.51
(1,1828)	1:43:A:LEU:HD12	1:48:A:ILE:H	2	0.51
(1,1828)	1:43:A:LEU:HD13	1:48:A:ILE:H	2	0.51
(1,1828)	1:43:A:LEU:HD21	1:48:A:ILE:H	2	0.51
(1,1828)	1:43:A:LEU:HD22	1:48:A:ILE:H	2	0.51
(1,1828)	1:43:A:LEU:HD23	1:48:A:ILE:H	2	0.51
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD11	3	0.51
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD12	3	0.51
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD13	3	0.51
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD21	3	0.51
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD22	3	0.51
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD23	3	0.51
(1,1690)	1:27:A:ARG:H	1:56:A:ARG:HD2	1	0.51
(1,1690)	1:27:A:ARG:H	1:56:A:ARG:HD3	1	0.51
(1,1640)	1:21:A:ARG:HB2	1:24:A:ASN:HB2	2	0.51
(1,1640)	1:21:A:ARG:HB2	1:24:A:ASN:HB3	2	0.51
(1,1640)	1:21:A:ARG:HB3	1:24:A:ASN:HB2	2	0.51
(1,1640)	1:21:A:ARG:HB3	1:24:A:ASN:HB3	2	0.51
(1,1180)	1:38:A:SER:HA	1:43:A:LEU:HG	1	0.51
(1,697)	1:11:A:PHE:HZ	1:51:A:TRP:HE1	1	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:42:A:GLY:H	1:43:A:LEU:HA	2	0.51
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD11	2	0.5
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD12	2	0.5
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD13	2	0.5
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD21	2	0.5
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD22	2	0.5
(1,1795)	1:38:A:SER:HA	1:43:A:LEU:HD23	2	0.5
(1,1740)	1:30:A:THR:HA	1:31:A:GLU:HG2	2	0.5
(1,1740)	1:30:A:THR:HA	1:31:A:GLU:HG3	2	0.5
(1,1630)	1:20:A:LYS:HG2	1:24:A:ASN:HD21	2	0.5
(1,1630)	1:20:A:LYS:HG2	1:24:A:ASN:HD22	2	0.5
(1,1630)	1:20:A:LYS:HG3	1:24:A:ASN:HD21	2	0.5
(1,1630)	1:20:A:LYS:HG3	1:24:A:ASN:HD22	2	0.5
(1,1628)	1:20:A:LYS:HA	1:24:A:ASN:HD21	2	0.5
(1,1628)	1:20:A:LYS:HA	1:24:A:ASN:HD22	2	0.5
(1,867)	1:38:A:SER:HB3	1:45:A:GLU:HA	1	0.5
(1,627)	1:9:A:THR:HA	1:11:A:PHE:HE1	2	0.5
(1,627)	1:9:A:THR:HA	1:11:A:PHE:HE2	2	0.5
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD21	2	0.5
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD22	2	0.5
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD23	2	0.5
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD21	3	0.5
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD22	3	0.5
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD23	3	0.5
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD11	3	0.5
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD12	3	0.5
(1,359)	1:44:A:ASN:H	1:48:A:ILE:HD13	3	0.5
(1,269)	1:11:A:PHE:H	1:11:A:PHE:HE1	3	0.5
(1,269)	1:11:A:PHE:H	1:11:A:PHE:HE2	3	0.5
(1,1828)	1:43:A:LEU:HD11	1:48:A:ILE:H	1	0.49
(1,1828)	1:43:A:LEU:HD12	1:48:A:ILE:H	1	0.49
(1,1828)	1:43:A:LEU:HD13	1:48:A:ILE:H	1	0.49
(1,1828)	1:43:A:LEU:HD21	1:48:A:ILE:H	1	0.49
(1,1828)	1:43:A:LEU:HD22	1:48:A:ILE:H	1	0.49
(1,1828)	1:43:A:LEU:HD23	1:48:A:ILE:H	1	0.49
(1,1286)	1:19:A:LEU:HA	1:20:A:LYS:HD2	3	0.49
(1,1286)	1:19:A:LEU:HA	1:20:A:LYS:HD3	3	0.49
(1,695)	1:11:A:PHE:HZ	1:47:A:GLN:H	2	0.49
(1,665)	1:23:A:PHE:HD1	1:55:A:GLU:HA	2	0.49
(1,665)	1:23:A:PHE:HD2	1:55:A:GLU:HA	2	0.49
(1,661)	1:23:A:PHE:HB3	1:51:A:TRP:HE3	3	0.49
(1,291)	1:34:A:ARG:HB3	1:45:A:GLU:H	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:10:A:ALA:H	1:47:A:GLN:HE22	3	0.49
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD11	3	0.48
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD12	3	0.48
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD13	3	0.48
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD21	3	0.48
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD22	3	0.48
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD23	3	0.48
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD11	3	0.48
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD12	3	0.48
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD13	3	0.48
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD21	3	0.48
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD22	3	0.48
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD23	3	0.48
(1,1734)	1:29:A:LEU:HD11	1:52:A:PHE:HA	1	0.48
(1,1734)	1:29:A:LEU:HD12	1:52:A:PHE:HA	1	0.48
(1,1734)	1:29:A:LEU:HD13	1:52:A:PHE:HA	1	0.48
(1,1734)	1:29:A:LEU:HD21	1:52:A:PHE:HA	1	0.48
(1,1734)	1:29:A:LEU:HD22	1:52:A:PHE:HA	1	0.48
(1,1734)	1:29:A:LEU:HD23	1:52:A:PHE:HA	1	0.48
(1,1731)	1:29:A:LEU:HD11	1:49:A:LYS:HB2	2	0.48
(1,1731)	1:29:A:LEU:HD12	1:49:A:LYS:HB2	2	0.48
(1,1731)	1:29:A:LEU:HD13	1:49:A:LYS:HB2	2	0.48
(1,1731)	1:29:A:LEU:HD21	1:49:A:LYS:HB2	2	0.48
(1,1731)	1:29:A:LEU:HD22	1:49:A:LYS:HB2	2	0.48
(1,1731)	1:29:A:LEU:HD23	1:49:A:LYS:HB2	2	0.48
(1,1634)	1:21:A:ARG:HA	1:24:A:ASN:HB2	3	0.48
(1,1634)	1:21:A:ARG:HA	1:24:A:ASN:HB3	3	0.48
(1,1301)	1:25:A:GLU:HG2	1:26:A:ASN:H	3	0.48
(1,1245)	1:37:A:LEU:HB2	1:48:A:ILE:HG12	2	0.48
(1,1245)	1:37:A:LEU:HB2	1:48:A:ILE:HG13	2	0.48
(1,1008)	1:20:A:LYS:H	1:20:A:LYS:HD2	2	0.48
(1,1008)	1:20:A:LYS:H	1:20:A:LYS:HD3	2	0.48
(1,903)	1:34:A:ARG:HD3	1:49:A:LYS:HD3	3	0.48
(1,762)	1:20:A:LYS:HA	1:51:A:TRP:HZ3	3	0.48
(1,753)	1:20:A:LYS:H	1:51:A:TRP:HZ2	1	0.48
(1,681)	1:39:A:SER:HA	1:43:A:LEU:H	1	0.48
(1,581)	1:17:A:ALA:HB1	1:18:A:ARG:H	3	0.48
(1,581)	1:17:A:ALA:HB2	1:18:A:ARG:H	3	0.48
(1,581)	1:17:A:ALA:HB3	1:18:A:ARG:H	3	0.48
(1,108)	1:10:A:ALA:H	1:47:A:GLN:HE22	1	0.48
(1,1911)	1:61:A:LYS:HA	1:61:A:LYS:HD2	2	0.47
(1,1911)	1:61:A:LYS:HA	1:61:A:LYS:HD3	2	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1013)	1:41:A:LEU:H	1:43:A:LEU:HG	2	0.47
(1,1013)	1:41:A:LEU:H	1:43:A:LEU:HG	3	0.47
(1,977)	1:37:A:LEU:HB3	1:48:A:ILE:HG21	1	0.47
(1,977)	1:37:A:LEU:HB3	1:48:A:ILE:HG22	1	0.47
(1,977)	1:37:A:LEU:HB3	1:48:A:ILE:HG23	1	0.47
(1,931)	1:27:A:ARG:HB2	1:56:A:ARG:HD3	2	0.47
(1,295)	1:13:A:SER:H	1:17:A:ALA:H	1	0.47
(1,294)	1:12:A:SER:H	1:16:A:LEU:H	3	0.47
(1,291)	1:34:A:ARG:HB3	1:45:A:GLU:H	2	0.47
(1,1815)	1:41:A:LEU:HD11	1:42:A:GLY:H	2	0.46
(1,1815)	1:41:A:LEU:HD12	1:42:A:GLY:H	2	0.46
(1,1815)	1:41:A:LEU:HD13	1:42:A:GLY:H	2	0.46
(1,1815)	1:41:A:LEU:HD21	1:42:A:GLY:H	2	0.46
(1,1815)	1:41:A:LEU:HD22	1:42:A:GLY:H	2	0.46
(1,1815)	1:41:A:LEU:HD23	1:42:A:GLY:H	2	0.46
(1,1690)	1:27:A:ARG:H	1:56:A:ARG:HD2	3	0.46
(1,1690)	1:27:A:ARG:H	1:56:A:ARG:HD3	3	0.46
(1,1367)	1:44:A:ASN:HD21	1:47:A:GLN:H	2	0.46
(1,1366)	1:56:A:ARG:H	1:56:A:ARG:HE	1	0.46
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG21	1	0.46
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG22	1	0.46
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG23	1	0.46
(1,820)	1:23:A:PHE:HZ	1:55:A:GLU:HA	2	0.46
(1,818)	1:48:A:ILE:HA	1:51:A:TRP:HD1	1	0.46
(1,530)	1:28:A:TYR:HD1	1:56:A:ARG:HE	2	0.46
(1,530)	1:28:A:TYR:HD2	1:56:A:ARG:HE	2	0.46
(1,495)	1:20:A:LYS:HB3	1:24:A:ASN:H	3	0.46
(1,295)	1:13:A:SER:H	1:17:A:ALA:H	2	0.46
(1,1854)	1:51:A:TRP:HA	1:54:A:ASN:HD21	1	0.45
(1,1854)	1:51:A:TRP:HA	1:54:A:ASN:HD22	1	0.45
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD11	2	0.45
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD12	2	0.45
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD13	2	0.45
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD21	2	0.45
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD22	2	0.45
(1,1797)	1:38:A:SER:HB2	1:41:A:LEU:HD23	2	0.45
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD11	2	0.45
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD12	2	0.45
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD13	2	0.45
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD21	2	0.45
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD22	2	0.45
(1,1797)	1:38:A:SER:HB3	1:41:A:LEU:HD23	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1734)	1:29:A:LEU:HD11	1:52:A:PHE:HA	2	0.45
(1,1734)	1:29:A:LEU:HD12	1:52:A:PHE:HA	2	0.45
(1,1734)	1:29:A:LEU:HD13	1:52:A:PHE:HA	2	0.45
(1,1734)	1:29:A:LEU:HD21	1:52:A:PHE:HA	2	0.45
(1,1734)	1:29:A:LEU:HD22	1:52:A:PHE:HA	2	0.45
(1,1734)	1:29:A:LEU:HD23	1:52:A:PHE:HA	2	0.45
(1,1730)	1:29:A:LEU:HD11	1:49:A:LYS:HA	2	0.45
(1,1730)	1:29:A:LEU:HD12	1:49:A:LYS:HA	2	0.45
(1,1730)	1:29:A:LEU:HD13	1:49:A:LYS:HA	2	0.45
(1,1730)	1:29:A:LEU:HD21	1:49:A:LYS:HA	2	0.45
(1,1730)	1:29:A:LEU:HD22	1:49:A:LYS:HA	2	0.45
(1,1730)	1:29:A:LEU:HD23	1:49:A:LYS:HA	2	0.45
(1,1225)	1:37:A:LEU:HG	1:52:A:PHE:HE1	2	0.45
(1,1225)	1:37:A:LEU:HG	1:52:A:PHE:HE2	2	0.45
(1,1052)	1:15:A:GLN:HE21	1:43:A:LEU:HD11	2	0.45
(1,1052)	1:15:A:GLN:HE21	1:43:A:LEU:HD12	2	0.45
(1,1052)	1:15:A:GLN:HE21	1:43:A:LEU:HD13	2	0.45
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG21	2	0.45
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG22	2	0.45
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG23	2	0.45
(1,297)	1:11:A:PHE:HE1	1:12:A:SER:H	1	0.45
(1,297)	1:11:A:PHE:HE2	1:12:A:SER:H	1	0.45
(1,1494)	1:6:A:ARG:HB2	1:7:A:PRO:HG2	3	0.44
(1,1494)	1:6:A:ARG:HB3	1:7:A:PRO:HG2	3	0.44
(1,1403)	1:23:A:PHE:HD1	1:27:A:ARG:H	2	0.44
(1,1403)	1:23:A:PHE:HD2	1:27:A:ARG:H	2	0.44
(1,1222)	1:57:A:ALA:HB1	1:58:A:LYS:H	1	0.44
(1,1222)	1:57:A:ALA:HB2	1:58:A:LYS:H	1	0.44
(1,1222)	1:57:A:ALA:HB3	1:58:A:LYS:H	1	0.44
(1,1012)	1:30:A:THR:HG21	1:32:A:ARG:H	2	0.44
(1,1012)	1:30:A:THR:HG22	1:32:A:ARG:H	2	0.44
(1,1012)	1:30:A:THR:HG23	1:32:A:ARG:H	2	0.44
(1,789)	1:19:A:LEU:HA	1:22:A:GLU:HA	1	0.44
(1,665)	1:23:A:PHE:HD1	1:55:A:GLU:HA	1	0.44
(1,665)	1:23:A:PHE:HD2	1:55:A:GLU:HA	1	0.44
(1,394)	1:44:A:ASN:HD21	1:46:A:ALA:H	2	0.44
(1,1839)	1:49:A:LYS:HA	1:49:A:LYS:HD2	3	0.43
(1,1839)	1:49:A:LYS:HA	1:49:A:LYS:HD3	3	0.43
(1,1472)	1:44:A:ASN:H	1:47:A:GLN:HE21	3	0.43
(1,1213)	1:28:A:TYR:HA	1:29:A:LEU:HB3	2	0.43
(1,1151)	1:15:A:GLN:HE21	1:41:A:LEU:HD21	3	0.43
(1,1151)	1:15:A:GLN:HE21	1:41:A:LEU:HD22	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:15:A:GLN:HE21	1:41:A:LEU:HD23	3	0.43
(1,1116)	1:59:A:ILE:HG21	1:61:A:LYS:HG3	1	0.43
(1,1116)	1:59:A:ILE:HG22	1:61:A:LYS:HG3	1	0.43
(1,1116)	1:59:A:ILE:HG23	1:61:A:LYS:HG3	1	0.43
(1,1012)	1:30:A:THR:HG21	1:32:A:ARG:H	3	0.43
(1,1012)	1:30:A:THR:HG22	1:32:A:ARG:H	3	0.43
(1,1012)	1:30:A:THR:HG23	1:32:A:ARG:H	3	0.43
(1,775)	1:55:A:GLU:HA	1:58:A:LYS:HG2	2	0.43
(1,762)	1:20:A:LYS:HA	1:51:A:TRP:HZ3	1	0.43
(1,665)	1:23:A:PHE:HD1	1:55:A:GLU:HA	3	0.43
(1,665)	1:23:A:PHE:HD2	1:55:A:GLU:HA	3	0.43
(1,490)	1:9:A:THR:HG21	1:11:A:PHE:H	2	0.43
(1,490)	1:9:A:THR:HG22	1:11:A:PHE:H	2	0.43
(1,490)	1:9:A:THR:HG23	1:11:A:PHE:H	2	0.43
(1,443)	1:38:A:SER:H	1:40:A:GLU:H	3	0.43
(1,298)	1:11:A:PHE:HD1	1:12:A:SER:H	3	0.43
(1,298)	1:11:A:PHE:HD2	1:12:A:SER:H	3	0.43
(1,1815)	1:41:A:LEU:HD11	1:42:A:GLY:H	3	0.42
(1,1815)	1:41:A:LEU:HD12	1:42:A:GLY:H	3	0.42
(1,1815)	1:41:A:LEU:HD13	1:42:A:GLY:H	3	0.42
(1,1815)	1:41:A:LEU:HD21	1:42:A:GLY:H	3	0.42
(1,1815)	1:41:A:LEU:HD22	1:42:A:GLY:H	3	0.42
(1,1815)	1:41:A:LEU:HD23	1:42:A:GLY:H	3	0.42
(1,1802)	1:38:A:SER:HB2	1:48:A:ILE:HG12	3	0.42
(1,1802)	1:38:A:SER:HB2	1:48:A:ILE:HG13	3	0.42
(1,1802)	1:38:A:SER:HB3	1:48:A:ILE:HG12	3	0.42
(1,1802)	1:38:A:SER:HB3	1:48:A:ILE:HG13	3	0.42
(1,1387)	1:54:A:ASN:HD22	1:55:A:GLU:HA	3	0.42
(1,1343)	1:22:A:GLU:HG2	1:37:A:LEU:H	1	0.42
(1,1343)	1:22:A:GLU:HG3	1:37:A:LEU:H	1	0.42
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB1	3	0.42
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB2	3	0.42
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB3	3	0.42
(1,1174)	1:19:A:LEU:HD21	1:41:A:LEU:HG	3	0.42
(1,1174)	1:19:A:LEU:HD22	1:41:A:LEU:HG	3	0.42
(1,1174)	1:19:A:LEU:HD23	1:41:A:LEU:HG	3	0.42
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD11	2	0.42
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD12	2	0.42
(1,1085)	1:33:A:ARG:HD3	1:37:A:LEU:HD13	2	0.42
(1,1065)	1:19:A:LEU:HD21	1:48:A:ILE:HB	1	0.42
(1,1065)	1:19:A:LEU:HD22	1:48:A:ILE:HB	1	0.42
(1,1065)	1:19:A:LEU:HD23	1:48:A:ILE:HB	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:18:A:ARG:HB2	1:37:A:LEU:HA	2	0.42
(1,891)	1:18:A:ARG:HB3	1:37:A:LEU:HA	2	0.42
(1,834)	1:30:A:THR:H	1:34:A:ARG:HD3	2	0.42
(1,490)	1:9:A:THR:HG21	1:11:A:PHE:H	1	0.42
(1,490)	1:9:A:THR:HG22	1:11:A:PHE:H	1	0.42
(1,490)	1:9:A:THR:HG23	1:11:A:PHE:H	1	0.42
(1,488)	1:29:A:LEU:HB3	1:34:A:ARG:HE	3	0.42
(1,422)	1:61:A:LYS:H	1:62:A:SER:HB2	2	0.42
(1,422)	1:61:A:LYS:H	1:62:A:SER:HB3	2	0.42
(1,347)	1:31:A:GLU:H	1:32:A:ARG:HA	1	0.42
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD11	1	0.42
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD12	1	0.42
(1,307)	1:12:A:SER:H	1:19:A:LEU:HD13	1	0.42
(1,262)	1:15:A:GLN:H	1:15:A:GLN:HE21	3	0.42
(1,35)	1:20:A:LYS:HG2	1:51:A:TRP:HH2	3	0.42
(1,35)	1:20:A:LYS:HG3	1:51:A:TRP:HH2	3	0.42
(1,1884)	1:56:A:ARG:H	1:58:A:LYS:HG2	2	0.41
(1,1884)	1:56:A:ARG:H	1:58:A:LYS:HG3	2	0.41
(1,1856)	1:51:A:TRP:HD1	1:54:A:ASN:HD21	2	0.41
(1,1856)	1:51:A:TRP:HD1	1:54:A:ASN:HD22	2	0.41
(1,1364)	1:30:A:THR:H	1:33:A:ARG:HE	1	0.41
(1,1173)	1:19:A:LEU:HD21	1:37:A:LEU:HG	3	0.41
(1,1173)	1:19:A:LEU:HD22	1:37:A:LEU:HG	3	0.41
(1,1173)	1:19:A:LEU:HD23	1:37:A:LEU:HG	3	0.41
(1,1050)	1:38:A:SER:HA	1:43:A:LEU:HD11	1	0.41
(1,1050)	1:38:A:SER:HA	1:43:A:LEU:HD12	1	0.41
(1,1050)	1:38:A:SER:HA	1:43:A:LEU:HD13	1	0.41
(1,888)	1:53:A:GLN:HG2	1:54:A:ASN:HA	2	0.41
(1,867)	1:38:A:SER:HB3	1:45:A:GLU:HA	2	0.41
(1,813)	1:15:A:GLN:HA	1:41:A:LEU:HA	2	0.41
(1,544)	1:42:A:GLY:H	1:43:A:LEU:HA	3	0.41
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG21	1	0.41
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG22	1	0.41
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG23	1	0.41
(1,381)	1:18:A:ARG:HE	1:22:A:GLU:HB2	2	0.41
(1,297)	1:11:A:PHE:HE1	1:12:A:SER:H	2	0.41
(1,297)	1:11:A:PHE:HE2	1:12:A:SER:H	2	0.41
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD11	1	0.4
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD12	1	0.4
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD13	1	0.4
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD21	1	0.4
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD22	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD23	1	0.4
(1,1750)	1:32:A:ARG:HB2	1:33:A:ARG:H	1	0.4
(1,1750)	1:32:A:ARG:HB3	1:33:A:ARG:H	1	0.4
(1,1690)	1:27:A:ARG:H	1:56:A:ARG:HD2	2	0.4
(1,1690)	1:27:A:ARG:H	1:56:A:ARG:HD3	2	0.4
(1,1366)	1:56:A:ARG:H	1:56:A:ARG:HE	3	0.4
(1,1284)	1:33:A:ARG:HD3	1:36:A:GLN:HB2	2	0.4
(1,764)	1:24:A:ASN:H	1:51:A:TRP:HZ3	1	0.4
(1,674)	1:23:A:PHE:HE1	1:56:A:ARG:HA	3	0.4
(1,674)	1:23:A:PHE:HE2	1:56:A:ARG:HA	3	0.4
(1,561)	1:22:A:GLU:HB2	1:52:A:PHE:HD1	3	0.4
(1,561)	1:22:A:GLU:HB2	1:52:A:PHE:HD2	3	0.4
(1,184)	1:8:A:ARG:HA	1:8:A:ARG:HD2	3	0.4
(1,184)	1:8:A:ARG:HA	1:8:A:ARG:HD3	3	0.4
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD11	3	0.39
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD12	3	0.39
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD13	3	0.39
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD21	3	0.39
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD22	3	0.39
(1,1819)	1:41:A:LEU:HD11	1:43:A:LEU:HD23	3	0.39
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD11	3	0.39
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD12	3	0.39
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD13	3	0.39
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD21	3	0.39
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD22	3	0.39
(1,1819)	1:41:A:LEU:HD12	1:43:A:LEU:HD23	3	0.39
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD11	3	0.39
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD12	3	0.39
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD13	3	0.39
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD21	3	0.39
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD22	3	0.39
(1,1819)	1:41:A:LEU:HD13	1:43:A:LEU:HD23	3	0.39
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD11	3	0.39
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD12	3	0.39
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD13	3	0.39
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD21	3	0.39
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD22	3	0.39
(1,1819)	1:41:A:LEU:HD21	1:43:A:LEU:HD23	3	0.39
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD11	3	0.39
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD12	3	0.39
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD13	3	0.39
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD21	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD22	3	0.39
(1,1819)	1:41:A:LEU:HD22	1:43:A:LEU:HD23	3	0.39
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD11	3	0.39
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD12	3	0.39
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD13	3	0.39
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD21	3	0.39
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD22	3	0.39
(1,1819)	1:41:A:LEU:HD23	1:43:A:LEU:HD23	3	0.39
(1,1818)	1:41:A:LEU:HD11	1:43:A:LEU:HG	1	0.39
(1,1818)	1:41:A:LEU:HD12	1:43:A:LEU:HG	1	0.39
(1,1818)	1:41:A:LEU:HD13	1:43:A:LEU:HG	1	0.39
(1,1818)	1:41:A:LEU:HD21	1:43:A:LEU:HG	1	0.39
(1,1818)	1:41:A:LEU:HD22	1:43:A:LEU:HG	1	0.39
(1,1818)	1:41:A:LEU:HD23	1:43:A:LEU:HG	1	0.39
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD11	1	0.39
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD12	1	0.39
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD13	1	0.39
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD21	1	0.39
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD22	1	0.39
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD23	1	0.39
(1,1712)	1:29:A:LEU:HD11	1:33:A:ARG:HD2	3	0.39
(1,1712)	1:29:A:LEU:HD11	1:33:A:ARG:HD3	3	0.39
(1,1712)	1:29:A:LEU:HD12	1:33:A:ARG:HD2	3	0.39
(1,1712)	1:29:A:LEU:HD12	1:33:A:ARG:HD3	3	0.39
(1,1712)	1:29:A:LEU:HD13	1:33:A:ARG:HD2	3	0.39
(1,1712)	1:29:A:LEU:HD13	1:33:A:ARG:HD3	3	0.39
(1,1712)	1:29:A:LEU:HD21	1:33:A:ARG:HD2	3	0.39
(1,1712)	1:29:A:LEU:HD21	1:33:A:ARG:HD3	3	0.39
(1,1712)	1:29:A:LEU:HD22	1:33:A:ARG:HD2	3	0.39
(1,1712)	1:29:A:LEU:HD22	1:33:A:ARG:HD3	3	0.39
(1,1712)	1:29:A:LEU:HD23	1:33:A:ARG:HD2	3	0.39
(1,1712)	1:29:A:LEU:HD23	1:33:A:ARG:HD3	3	0.39
(1,1494)	1:6:A:ARG:HB2	1:7:A:PRO:HG2	2	0.39
(1,1494)	1:6:A:ARG:HB3	1:7:A:PRO:HG2	2	0.39
(1,1418)	1:11:A:PHE:HB2	1:16:A:LEU:HB3	3	0.39
(1,901)	1:6:A:ARG:HD2	1:7:A:PRO:HD3	3	0.39
(1,901)	1:6:A:ARG:HD3	1:7:A:PRO:HD3	3	0.39
(1,760)	1:24:A:ASN:H	1:51:A:TRP:HH2	2	0.39
(1,717)	1:50:A:ILE:HG21	1:51:A:TRP:HD1	1	0.39
(1,717)	1:50:A:ILE:HG22	1:51:A:TRP:HD1	1	0.39
(1,717)	1:50:A:ILE:HG23	1:51:A:TRP:HD1	1	0.39
(1,689)	1:23:A:PHE:HE1	1:27:A:ARG:H	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,689)	1:23:A:PHE:HE2	1:27:A:ARG:H	2	0.39
(1,617)	1:34:A:ARG:HD2	1:48:A:ILE:H	3	0.39
(1,609)	1:11:A:PHE:HD1	1:16:A:LEU:HB2	1	0.39
(1,609)	1:11:A:PHE:HD2	1:16:A:LEU:HB2	1	0.39
(1,526)	1:23:A:PHE:HZ	1:55:A:GLU:H	1	0.39
(1,315)	1:44:A:ASN:H	1:47:A:GLN:HB3	1	0.39
(1,1770)	1:34:A:ARG:HD3	1:49:A:LYS:HD2	1	0.38
(1,1770)	1:34:A:ARG:HD3	1:49:A:LYS:HD3	1	0.38
(1,1699)	1:27:A:ARG:HG2	1:56:A:ARG:HD2	3	0.38
(1,1699)	1:27:A:ARG:HG2	1:56:A:ARG:HD3	3	0.38
(1,1699)	1:27:A:ARG:HG3	1:56:A:ARG:HD2	3	0.38
(1,1699)	1:27:A:ARG:HG3	1:56:A:ARG:HD3	3	0.38
(1,1482)	1:11:A:PHE:HB2	1:16:A:LEU:HB2	3	0.38
(1,1432)	1:47:A:GLN:H	1:49:A:LYS:HB3	1	0.38
(1,1328)	1:28:A:TYR:HE1	1:53:A:GLN:HG3	3	0.38
(1,1328)	1:28:A:TYR:HE2	1:53:A:GLN:HG3	3	0.38
(1,1233)	1:30:A:THR:HG21	1:34:A:ARG:H	3	0.38
(1,1233)	1:30:A:THR:HG22	1:34:A:ARG:H	3	0.38
(1,1233)	1:30:A:THR:HG23	1:34:A:ARG:H	3	0.38
(1,1213)	1:28:A:TYR:HA	1:29:A:LEU:HB3	3	0.38
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD11	3	0.38
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD12	3	0.38
(1,1155)	1:47:A:GLN:HE21	1:50:A:ILE:HD13	3	0.38
(1,1064)	1:19:A:LEU:HD21	1:22:A:GLU:HB3	2	0.38
(1,1064)	1:19:A:LEU:HD22	1:22:A:GLU:HB3	2	0.38
(1,1064)	1:19:A:LEU:HD23	1:22:A:GLU:HB3	2	0.38
(1,832)	1:53:A:GLN:HA	1:53:A:GLN:HE22	3	0.38
(1,707)	1:29:A:LEU:HD21	1:51:A:TRP:HE3	2	0.38
(1,707)	1:29:A:LEU:HD22	1:51:A:TRP:HE3	2	0.38
(1,707)	1:29:A:LEU:HD23	1:51:A:TRP:HE3	2	0.38
(1,661)	1:23:A:PHE:HB3	1:51:A:TRP:HE3	1	0.38
(1,655)	1:10:A:ALA:HB1	1:11:A:PHE:HE1	3	0.38
(1,655)	1:10:A:ALA:HB1	1:11:A:PHE:HE2	3	0.38
(1,655)	1:10:A:ALA:HB2	1:11:A:PHE:HE1	3	0.38
(1,655)	1:10:A:ALA:HB2	1:11:A:PHE:HE2	3	0.38
(1,655)	1:10:A:ALA:HB3	1:11:A:PHE:HE1	3	0.38
(1,655)	1:10:A:ALA:HB3	1:11:A:PHE:HE2	3	0.38
(1,561)	1:22:A:GLU:HB2	1:52:A:PHE:HD1	2	0.38
(1,561)	1:22:A:GLU:HB2	1:52:A:PHE:HD2	2	0.38
(1,530)	1:28:A:TYR:HD1	1:56:A:ARG:HE	3	0.38
(1,530)	1:28:A:TYR:HD2	1:56:A:ARG:HE	3	0.38
(1,405)	1:29:A:LEU:HA	1:34:A:ARG:H	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:28:A:TYR:H	1:28:A:TYR:HD1	2	0.38
(1,118)	1:28:A:TYR:H	1:28:A:TYR:HD2	2	0.38
(1,1855)	1:51:A:TRP:HB2	1:54:A:ASN:HD21	1	0.37
(1,1855)	1:51:A:TRP:HB2	1:54:A:ASN:HD22	1	0.37
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD11	1	0.37
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD12	1	0.37
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD13	1	0.37
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD21	1	0.37
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD22	1	0.37
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD23	1	0.37
(1,1738)	1:29:A:LEU:HD11	1:53:A:GLN:H	1	0.37
(1,1738)	1:29:A:LEU:HD12	1:53:A:GLN:H	1	0.37
(1,1738)	1:29:A:LEU:HD13	1:53:A:GLN:H	1	0.37
(1,1738)	1:29:A:LEU:HD21	1:53:A:GLN:H	1	0.37
(1,1738)	1:29:A:LEU:HD22	1:53:A:GLN:H	1	0.37
(1,1738)	1:29:A:LEU:HD23	1:53:A:GLN:H	1	0.37
(1,1699)	1:27:A:ARG:HG2	1:56:A:ARG:HD2	1	0.37
(1,1699)	1:27:A:ARG:HG2	1:56:A:ARG:HD3	1	0.37
(1,1699)	1:27:A:ARG:HG3	1:56:A:ARG:HD2	1	0.37
(1,1699)	1:27:A:ARG:HG3	1:56:A:ARG:HD3	1	0.37
(1,1630)	1:20:A:LYS:HG2	1:24:A:ASN:HD21	1	0.37
(1,1630)	1:20:A:LYS:HG2	1:24:A:ASN:HD22	1	0.37
(1,1630)	1:20:A:LYS:HG3	1:24:A:ASN:HD21	1	0.37
(1,1630)	1:20:A:LYS:HG3	1:24:A:ASN:HD22	1	0.37
(1,1287)	1:19:A:LEU:HA	1:22:A:GLU:HB3	1	0.37
(1,1042)	1:29:A:LEU:HD11	1:30:A:THR:H	2	0.37
(1,1042)	1:29:A:LEU:HD12	1:30:A:THR:H	2	0.37
(1,1042)	1:29:A:LEU:HD13	1:30:A:THR:H	2	0.37
(1,834)	1:30:A:THR:H	1:34:A:ARG:HD3	1	0.37
(1,777)	1:15:A:GLN:HA	1:19:A:LEU:HG	3	0.37
(1,717)	1:50:A:ILE:HG21	1:51:A:TRP:HD1	2	0.37
(1,717)	1:50:A:ILE:HG22	1:51:A:TRP:HD1	2	0.37
(1,717)	1:50:A:ILE:HG23	1:51:A:TRP:HD1	2	0.37
(1,717)	1:50:A:ILE:HG21	1:51:A:TRP:HD1	3	0.37
(1,717)	1:50:A:ILE:HG22	1:51:A:TRP:HD1	3	0.37
(1,717)	1:50:A:ILE:HG23	1:51:A:TRP:HD1	3	0.37
(1,705)	1:23:A:PHE:HZ	1:55:A:GLU:HB2	3	0.37
(1,674)	1:23:A:PHE:HE1	1:56:A:ARG:HA	1	0.37
(1,674)	1:23:A:PHE:HE2	1:56:A:ARG:HA	1	0.37
(1,455)	1:49:A:LYS:HD2	1:50:A:ILE:H	2	0.37
(1,411)	1:19:A:LEU:HD11	1:51:A:TRP:H	1	0.37
(1,411)	1:19:A:LEU:HD12	1:51:A:TRP:H	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:19:A:LEU:HD13	1:51:A:TRP:H	1	0.37
(1,405)	1:29:A:LEU:HA	1:34:A:ARG:H	3	0.37
(1,381)	1:18:A:ARG:HE	1:22:A:GLU:HB2	1	0.37
(1,364)	1:48:A:ILE:HB	1:52:A:PHE:H	1	0.37
(1,1712)	1:29:A:LEU:HD11	1:33:A:ARG:HD2	2	0.36
(1,1712)	1:29:A:LEU:HD11	1:33:A:ARG:HD3	2	0.36
(1,1712)	1:29:A:LEU:HD12	1:33:A:ARG:HD2	2	0.36
(1,1712)	1:29:A:LEU:HD12	1:33:A:ARG:HD3	2	0.36
(1,1712)	1:29:A:LEU:HD13	1:33:A:ARG:HD2	2	0.36
(1,1712)	1:29:A:LEU:HD13	1:33:A:ARG:HD3	2	0.36
(1,1712)	1:29:A:LEU:HD21	1:33:A:ARG:HD2	2	0.36
(1,1712)	1:29:A:LEU:HD21	1:33:A:ARG:HD3	2	0.36
(1,1712)	1:29:A:LEU:HD22	1:33:A:ARG:HD2	2	0.36
(1,1712)	1:29:A:LEU:HD22	1:33:A:ARG:HD3	2	0.36
(1,1712)	1:29:A:LEU:HD23	1:33:A:ARG:HD2	2	0.36
(1,1712)	1:29:A:LEU:HD23	1:33:A:ARG:HD3	2	0.36
(1,1669)	1:24:A:ASN:HD21	1:25:A:GLU:HA	2	0.36
(1,1669)	1:24:A:ASN:HD22	1:25:A:GLU:HA	2	0.36
(1,1662)	1:24:A:ASN:H	1:24:A:ASN:HD21	3	0.36
(1,1662)	1:24:A:ASN:H	1:24:A:ASN:HD22	3	0.36
(1,1628)	1:20:A:LYS:HA	1:24:A:ASN:HD21	1	0.36
(1,1628)	1:20:A:LYS:HA	1:24:A:ASN:HD22	1	0.36
(1,1412)	1:51:A:TRP:HH2	1:55:A:GLU:HG3	2	0.36
(1,1404)	1:34:A:ARG:HD3	1:45:A:GLU:HA	2	0.36
(1,1354)	1:11:A:PHE:HB2	1:12:A:SER:HA	1	0.36
(1,1252)	1:34:A:ARG:HB3	1:48:A:ILE:HB	2	0.36
(1,1186)	1:11:A:PHE:HE1	1:43:A:LEU:HG	2	0.36
(1,1186)	1:11:A:PHE:HE2	1:43:A:LEU:HG	2	0.36
(1,1157)	1:50:A:ILE:HG21	1:53:A:GLN:HE22	3	0.36
(1,1157)	1:50:A:ILE:HG22	1:53:A:GLN:HE22	3	0.36
(1,1157)	1:50:A:ILE:HG23	1:53:A:GLN:HE22	3	0.36
(1,1101)	1:18:A:ARG:H	1:19:A:LEU:HB2	2	0.36
(1,1101)	1:18:A:ARG:H	1:19:A:LEU:HB3	2	0.36
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD11	1	0.36
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD12	1	0.36
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD13	1	0.36
(1,1056)	1:43:A:LEU:HD11	1:47:A:GLN:HE22	3	0.36
(1,1056)	1:43:A:LEU:HD12	1:47:A:GLN:HE22	3	0.36
(1,1056)	1:43:A:LEU:HD13	1:47:A:GLN:HE22	3	0.36
(1,888)	1:53:A:GLN:HG2	1:54:A:ASN:HA	3	0.36
(1,818)	1:48:A:ILE:HA	1:51:A:TRP:HD1	3	0.36
(1,789)	1:19:A:LEU:HA	1:22:A:GLU:HA	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,716)	1:50:A:ILE:HD11	1:53:A:GLN:HE21	1	0.36
(1,716)	1:50:A:ILE:HD12	1:53:A:GLN:HE21	1	0.36
(1,716)	1:50:A:ILE:HD13	1:53:A:GLN:HE21	1	0.36
(1,693)	1:24:A:ASN:H	1:52:A:PHE:HZ	1	0.36
(1,561)	1:22:A:GLU:HB2	1:52:A:PHE:HD1	1	0.36
(1,561)	1:22:A:GLU:HB2	1:52:A:PHE:HD2	1	0.36
(1,542)	1:44:A:ASN:HD21	1:47:A:GLN:HG2	1	0.36
(1,471)	1:13:A:SER:HA	1:17:A:ALA:H	3	0.36
(1,463)	1:51:A:TRP:HE3	1:53:A:GLN:H	1	0.36
(1,364)	1:48:A:ILE:HB	1:52:A:PHE:H	2	0.36
(1,270)	1:11:A:PHE:HA	1:11:A:PHE:HE1	3	0.36
(1,270)	1:11:A:PHE:HA	1:11:A:PHE:HE2	3	0.36
(1,189)	1:44:A:ASN:HA	1:44:A:ASN:HD21	2	0.36
(1,1911)	1:61:A:LYS:HA	1:61:A:LYS:HD2	1	0.35
(1,1911)	1:61:A:LYS:HA	1:61:A:LYS:HD3	1	0.35
(1,1911)	1:61:A:LYS:HA	1:61:A:LYS:HD2	3	0.35
(1,1911)	1:61:A:LYS:HA	1:61:A:LYS:HD3	3	0.35
(1,1666)	1:24:A:ASN:HB2	1:25:A:GLU:H	3	0.35
(1,1666)	1:24:A:ASN:HB3	1:25:A:GLU:H	3	0.35
(1,1514)	1:11:A:PHE:HB2	1:15:A:GLN:HB2	3	0.35
(1,1514)	1:11:A:PHE:HB2	1:15:A:GLN:HB3	3	0.35
(1,1505)	1:8:A:ARG:HB2	1:9:A:THR:HG21	1	0.35
(1,1505)	1:8:A:ARG:HB2	1:9:A:THR:HG22	1	0.35
(1,1505)	1:8:A:ARG:HB2	1:9:A:THR:HG23	1	0.35
(1,1505)	1:8:A:ARG:HB3	1:9:A:THR:HG21	1	0.35
(1,1505)	1:8:A:ARG:HB3	1:9:A:THR:HG22	1	0.35
(1,1505)	1:8:A:ARG:HB3	1:9:A:THR:HG23	1	0.35
(1,1403)	1:23:A:PHE:HD1	1:27:A:ARG:H	1	0.35
(1,1403)	1:23:A:PHE:HD2	1:27:A:ARG:H	1	0.35
(1,1373)	1:23:A:PHE:HE1	1:27:A:ARG:HD2	3	0.35
(1,1373)	1:23:A:PHE:HE2	1:27:A:ARG:HD2	3	0.35
(1,1363)	1:18:A:ARG:H	1:21:A:ARG:H	1	0.35
(1,1252)	1:34:A:ARG:HB3	1:48:A:ILE:HB	1	0.35
(1,1047)	1:29:A:LEU:HD21	1:52:A:PHE:HB2	3	0.35
(1,1047)	1:29:A:LEU:HD22	1:52:A:PHE:HB2	3	0.35
(1,1047)	1:29:A:LEU:HD23	1:52:A:PHE:HB2	3	0.35
(1,650)	1:23:A:PHE:HE1	1:55:A:GLU:HB2	3	0.35
(1,650)	1:23:A:PHE:HE2	1:55:A:GLU:HB2	3	0.35
(1,627)	1:9:A:THR:HA	1:11:A:PHE:HE1	3	0.35
(1,627)	1:9:A:THR:HA	1:11:A:PHE:HE2	3	0.35
(1,441)	1:16:A:LEU:H	1:18:A:ARG:H	1	0.35
(1,273)	1:11:A:PHE:HZ	1:51:A:TRP:HD1	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1666)	1:24:A:ASN:HB2	1:25:A:GLU:H	2	0.34
(1,1666)	1:24:A:ASN:HB3	1:25:A:GLU:H	2	0.34
(1,1640)	1:21:A:ARG:HB2	1:24:A:ASN:HB2	3	0.34
(1,1640)	1:21:A:ARG:HB2	1:24:A:ASN:HB3	3	0.34
(1,1640)	1:21:A:ARG:HB3	1:24:A:ASN:HB2	3	0.34
(1,1640)	1:21:A:ARG:HB3	1:24:A:ASN:HB3	3	0.34
(1,1587)	1:16:A:LEU:HD11	1:19:A:LEU:HA	1	0.34
(1,1587)	1:16:A:LEU:HD12	1:19:A:LEU:HA	1	0.34
(1,1587)	1:16:A:LEU:HD13	1:19:A:LEU:HA	1	0.34
(1,1587)	1:16:A:LEU:HD21	1:19:A:LEU:HA	1	0.34
(1,1587)	1:16:A:LEU:HD22	1:19:A:LEU:HA	1	0.34
(1,1587)	1:16:A:LEU:HD23	1:19:A:LEU:HA	1	0.34
(1,1377)	1:49:A:LYS:HB2	1:50:A:ILE:HA	3	0.34
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB1	2	0.34
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB2	2	0.34
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB3	2	0.34
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG21	2	0.34
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG22	2	0.34
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG23	2	0.34
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD11	1	0.34
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD12	1	0.34
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD13	1	0.34
(1,962)	1:45:A:GLU:HA	1:45:A:GLU:HG2	3	0.34
(1,891)	1:18:A:ARG:HB2	1:37:A:LEU:HA	1	0.34
(1,891)	1:18:A:ARG:HB3	1:37:A:LEU:HA	1	0.34
(1,789)	1:19:A:LEU:HA	1:22:A:GLU:HA	3	0.34
(1,783)	1:6:A:ARG:HB3	1:7:A:PRO:HD3	3	0.34
(1,779)	1:55:A:GLU:HA	1:58:A:LYS:HB3	1	0.34
(1,695)	1:11:A:PHE:HZ	1:47:A:GLN:H	1	0.34
(1,526)	1:23:A:PHE:HZ	1:55:A:GLU:H	3	0.34
(1,454)	1:8:A:ARG:HG2	1:9:A:THR:H	1	0.34
(1,422)	1:61:A:LYS:H	1:62:A:SER:HB2	1	0.34
(1,422)	1:61:A:LYS:H	1:62:A:SER:HB3	1	0.34
(1,357)	1:44:A:ASN:H	1:47:A:GLN:HG2	3	0.34
(1,346)	1:44:A:ASN:H	1:47:A:GLN:HA	2	0.34
(1,1640)	1:21:A:ARG:HB2	1:24:A:ASN:HB2	1	0.33
(1,1640)	1:21:A:ARG:HB2	1:24:A:ASN:HB3	1	0.33
(1,1640)	1:21:A:ARG:HB3	1:24:A:ASN:HB2	1	0.33
(1,1640)	1:21:A:ARG:HB3	1:24:A:ASN:HB3	1	0.33
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD11	1	0.33
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD12	1	0.33
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD13	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD21	1	0.33
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD22	1	0.33
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD23	1	0.33
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD11	1	0.33
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD12	1	0.33
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD13	1	0.33
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD21	1	0.33
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD22	1	0.33
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD23	1	0.33
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD11	1	0.33
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD12	1	0.33
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD13	1	0.33
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD21	1	0.33
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD22	1	0.33
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD23	1	0.33
(1,1514)	1:11:A:PHE:HB2	1:15:A:GLN:HB2	1	0.33
(1,1514)	1:11:A:PHE:HB2	1:15:A:GLN:HB3	1	0.33
(1,1437)	1:15:A:GLN:HA	1:19:A:LEU:H	3	0.33
(1,1406)	1:51:A:TRP:HB2	1:52:A:PHE:HA	3	0.33
(1,1256)	1:34:A:ARG:HA	1:48:A:ILE:HB	1	0.33
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD21	1	0.33
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD22	1	0.33
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD23	1	0.33
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG21	3	0.33
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG22	3	0.33
(1,1168)	1:37:A:LEU:HG	1:48:A:ILE:HG23	3	0.33
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD21	3	0.33
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD22	3	0.33
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD23	3	0.33
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD21	3	0.33
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD22	3	0.33
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD23	3	0.33
(1,861)	1:53:A:GLN:HA	1:56:A:ARG:HH11	3	0.33
(1,795)	1:5:A:LYS:HA	1:6:A:ARG:HD2	1	0.33
(1,795)	1:5:A:LYS:HA	1:6:A:ARG:HD3	1	0.33
(1,564)	1:47:A:GLN:HA	1:47:A:GLN:HE21	2	0.33
(1,521)	1:53:A:GLN:HA	1:55:A:GLU:H	1	0.33
(1,467)	1:54:A:ASN:HD22	1:55:A:GLU:H	3	0.33
(1,467)	1:54:A:ASN:HD21	1:55:A:GLU:H	3	0.33
(1,381)	1:18:A:ARG:HE	1:22:A:GLU:HB2	3	0.33
(1,293)	1:11:A:PHE:HE1	1:51:A:TRP:HE1	1	0.33
(1,293)	1:11:A:PHE:HE2	1:51:A:TRP:HE1	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:41:A:LEU:H	1:41:A:LEU:HD21	1	0.33
(1,225)	1:41:A:LEU:H	1:41:A:LEU:HD22	1	0.33
(1,225)	1:41:A:LEU:H	1:41:A:LEU:HD23	1	0.33
(1,204)	1:41:A:LEU:HB2	1:43:A:LEU:H	2	0.33
(1,102)	1:29:A:LEU:HA	1:33:A:ARG:HE	1	0.33
(1,1734)	1:29:A:LEU:HD11	1:52:A:PHE:HA	3	0.32
(1,1734)	1:29:A:LEU:HD12	1:52:A:PHE:HA	3	0.32
(1,1734)	1:29:A:LEU:HD13	1:52:A:PHE:HA	3	0.32
(1,1734)	1:29:A:LEU:HD21	1:52:A:PHE:HA	3	0.32
(1,1734)	1:29:A:LEU:HD22	1:52:A:PHE:HA	3	0.32
(1,1734)	1:29:A:LEU:HD23	1:52:A:PHE:HA	3	0.32
(1,1463)	1:11:A:PHE:HB3	1:15:A:GLN:H	3	0.32
(1,1355)	1:33:A:ARG:H	1:35:A:GLN:HB3	1	0.32
(1,1354)	1:11:A:PHE:HB2	1:12:A:SER:HA	3	0.32
(1,1287)	1:19:A:LEU:HA	1:22:A:GLU:HB3	2	0.32
(1,1157)	1:50:A:ILE:HG21	1:53:A:GLN:HE22	2	0.32
(1,1157)	1:50:A:ILE:HG22	1:53:A:GLN:HE22	2	0.32
(1,1157)	1:50:A:ILE:HG23	1:53:A:GLN:HE22	2	0.32
(1,1008)	1:20:A:LYS:H	1:20:A:LYS:HD2	1	0.32
(1,1008)	1:20:A:LYS:H	1:20:A:LYS:HD3	1	0.32
(1,768)	1:29:A:LEU:HG	1:34:A:ARG:HA	3	0.32
(1,601)	1:20:A:LYS:HG2	1:51:A:TRP:HZ2	1	0.32
(1,601)	1:20:A:LYS:HG3	1:51:A:TRP:HZ2	1	0.32
(1,463)	1:51:A:TRP:HE3	1:53:A:GLN:H	2	0.32
(1,405)	1:29:A:LEU:HA	1:34:A:ARG:H	2	0.32
(1,348)	1:49:A:LYS:HA	1:52:A:PHE:H	3	0.32
(1,347)	1:31:A:GLU:H	1:32:A:ARG:HA	2	0.32
(1,319)	1:44:A:ASN:HD22	1:45:A:GLU:H	2	0.32
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB1	1	0.32
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB2	1	0.32
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB3	1	0.32
(1,293)	1:11:A:PHE:HE1	1:51:A:TRP:HE1	3	0.32
(1,293)	1:11:A:PHE:HE2	1:51:A:TRP:HE1	3	0.32
(1,95)	1:22:A:GLU:H	1:23:A:PHE:HB3	2	0.32
(1,49)	1:34:A:ARG:H	1:36:A:GLN:H	3	0.32
(1,20)	1:15:A:GLN:HA	1:15:A:GLN:HE21	3	0.32
(1,1818)	1:41:A:LEU:HD11	1:43:A:LEU:HG	2	0.31
(1,1818)	1:41:A:LEU:HD12	1:43:A:LEU:HG	2	0.31
(1,1818)	1:41:A:LEU:HD13	1:43:A:LEU:HG	2	0.31
(1,1818)	1:41:A:LEU:HD21	1:43:A:LEU:HG	2	0.31
(1,1818)	1:41:A:LEU:HD22	1:43:A:LEU:HG	2	0.31
(1,1818)	1:41:A:LEU:HD23	1:43:A:LEU:HG	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1514)	1:11:A:PHE:HB2	1:15:A:GLN:HB2	2	0.31
(1,1514)	1:11:A:PHE:HB2	1:15:A:GLN:HB3	2	0.31
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD11	1	0.31
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD12	1	0.31
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD13	1	0.31
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD21	1	0.31
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD22	1	0.31
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD23	1	0.31
(1,1406)	1:51:A:TRP:HB2	1:52:A:PHE:HA	2	0.31
(1,1398)	1:17:A:ALA:H	1:19:A:LEU:HD11	2	0.31
(1,1398)	1:17:A:ALA:H	1:19:A:LEU:HD12	2	0.31
(1,1398)	1:17:A:ALA:H	1:19:A:LEU:HD13	2	0.31
(1,1394)	1:11:A:PHE:HD1	1:16:A:LEU:HB3	1	0.31
(1,1394)	1:11:A:PHE:HD2	1:16:A:LEU:HB3	1	0.31
(1,1328)	1:28:A:TYR:HE1	1:53:A:GLN:HG3	1	0.31
(1,1328)	1:28:A:TYR:HE2	1:53:A:GLN:HG3	1	0.31
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD11	2	0.31
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD12	2	0.31
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD13	2	0.31
(1,1186)	1:11:A:PHE:HE1	1:43:A:LEU:HG	3	0.31
(1,1186)	1:11:A:PHE:HE2	1:43:A:LEU:HG	3	0.31
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG21	1	0.31
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG22	1	0.31
(1,1153)	1:11:A:PHE:HZ	1:48:A:ILE:HG23	1	0.31
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD11	2	0.31
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD12	2	0.31
(1,1074)	1:45:A:GLU:HG2	1:48:A:ILE:HD13	2	0.31
(1,1053)	1:23:A:PHE:HD1	1:55:A:GLU:HB2	3	0.31
(1,1053)	1:23:A:PHE:HD2	1:55:A:GLU:HB2	3	0.31
(1,832)	1:53:A:GLN:HA	1:53:A:GLN:HE22	1	0.31
(1,813)	1:15:A:GLN:HA	1:41:A:LEU:HA	3	0.31
(1,755)	1:51:A:TRP:HD1	1:52:A:PHE:H	1	0.31
(1,693)	1:24:A:ASN:H	1:52:A:PHE:HZ	2	0.31
(1,654)	1:48:A:ILE:HG21	1:51:A:TRP:HE3	1	0.31
(1,654)	1:48:A:ILE:HG22	1:51:A:TRP:HE3	1	0.31
(1,654)	1:48:A:ILE:HG23	1:51:A:TRP:HE3	1	0.31
(1,627)	1:9:A:THR:HA	1:11:A:PHE:HE1	1	0.31
(1,627)	1:9:A:THR:HA	1:11:A:PHE:HE2	1	0.31
(1,575)	1:29:A:LEU:HG	1:30:A:THR:H	3	0.31
(1,508)	1:19:A:LEU:HD11	1:52:A:PHE:HD1	1	0.31
(1,508)	1:19:A:LEU:HD11	1:52:A:PHE:HD2	1	0.31
(1,508)	1:19:A:LEU:HD12	1:52:A:PHE:HD1	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:19:A:LEU:HD12	1:52:A:PHE:HD2	1	0.31
(1,508)	1:19:A:LEU:HD13	1:52:A:PHE:HD1	1	0.31
(1,508)	1:19:A:LEU:HD13	1:52:A:PHE:HD2	1	0.31
(1,449)	1:23:A:PHE:HZ	1:56:A:ARG:H	2	0.31
(1,372)	1:44:A:ASN:H	1:46:A:ALA:H	1	0.31
(1,319)	1:44:A:ASN:HD22	1:45:A:GLU:H	1	0.31
(1,1687)	1:26:A:ASN:HD21	1:27:A:ARG:H	3	0.3
(1,1687)	1:26:A:ASN:HD22	1:27:A:ARG:H	3	0.3
(1,1492)	1:5:A:LYS:HB2	1:6:A:ARG:H	3	0.3
(1,1492)	1:5:A:LYS:HB3	1:6:A:ARG:H	3	0.3
(1,1463)	1:11:A:PHE:HB3	1:15:A:GLN:H	1	0.3
(1,1459)	1:19:A:LEU:HD11	1:48:A:ILE:HA	1	0.3
(1,1459)	1:19:A:LEU:HD12	1:48:A:ILE:HA	1	0.3
(1,1459)	1:19:A:LEU:HD13	1:48:A:ILE:HA	1	0.3
(1,1418)	1:11:A:PHE:HB2	1:16:A:LEU:HB3	2	0.3
(1,1341)	1:56:A:ARG:H	1:56:A:ARG:HD2	2	0.3
(1,1287)	1:19:A:LEU:HA	1:22:A:GLU:HB3	3	0.3
(1,1225)	1:37:A:LEU:HG	1:52:A:PHE:HE1	1	0.3
(1,1225)	1:37:A:LEU:HG	1:52:A:PHE:HE2	1	0.3
(1,1172)	1:19:A:LEU:HD11	1:48:A:ILE:HG21	1	0.3
(1,1172)	1:19:A:LEU:HD11	1:48:A:ILE:HG22	1	0.3
(1,1172)	1:19:A:LEU:HD11	1:48:A:ILE:HG23	1	0.3
(1,1172)	1:19:A:LEU:HD12	1:48:A:ILE:HG21	1	0.3
(1,1172)	1:19:A:LEU:HD12	1:48:A:ILE:HG22	1	0.3
(1,1172)	1:19:A:LEU:HD12	1:48:A:ILE:HG23	1	0.3
(1,1172)	1:19:A:LEU:HD13	1:48:A:ILE:HG21	1	0.3
(1,1172)	1:19:A:LEU:HD13	1:48:A:ILE:HG22	1	0.3
(1,1172)	1:19:A:LEU:HD13	1:48:A:ILE:HG23	1	0.3
(1,1172)	1:19:A:LEU:HD11	1:48:A:ILE:HG21	3	0.3
(1,1172)	1:19:A:LEU:HD11	1:48:A:ILE:HG22	3	0.3
(1,1172)	1:19:A:LEU:HD11	1:48:A:ILE:HG23	3	0.3
(1,1172)	1:19:A:LEU:HD12	1:48:A:ILE:HG21	3	0.3
(1,1172)	1:19:A:LEU:HD12	1:48:A:ILE:HG22	3	0.3
(1,1172)	1:19:A:LEU:HD12	1:48:A:ILE:HG23	3	0.3
(1,1172)	1:19:A:LEU:HD13	1:48:A:ILE:HG21	3	0.3
(1,1172)	1:19:A:LEU:HD13	1:48:A:ILE:HG22	3	0.3
(1,1172)	1:19:A:LEU:HD13	1:48:A:ILE:HG23	3	0.3
(1,1043)	1:29:A:LEU:HD11	1:33:A:ARG:HE	3	0.3
(1,1043)	1:29:A:LEU:HD12	1:33:A:ARG:HE	3	0.3
(1,1043)	1:29:A:LEU:HD13	1:33:A:ARG:HE	3	0.3
(1,821)	1:23:A:PHE:HB3	1:51:A:TRP:HZ2	2	0.3
(1,713)	1:11:A:PHE:HD1	1:16:A:LEU:HD11	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,713)	1:11:A:PHE:HD1	1:16:A:LEU:HD12	1	0.3
(1,713)	1:11:A:PHE:HD1	1:16:A:LEU:HD13	1	0.3
(1,713)	1:11:A:PHE:HD2	1:16:A:LEU:HD11	1	0.3
(1,713)	1:11:A:PHE:HD2	1:16:A:LEU:HD12	1	0.3
(1,713)	1:11:A:PHE:HD2	1:16:A:LEU:HD13	1	0.3
(1,630)	1:51:A:TRP:HH2	1:52:A:PHE:HE1	2	0.3
(1,630)	1:51:A:TRP:HH2	1:52:A:PHE:HE2	2	0.3
(1,583)	1:29:A:LEU:HB3	1:52:A:PHE:HD1	2	0.3
(1,583)	1:29:A:LEU:HB3	1:52:A:PHE:HD2	2	0.3
(1,583)	1:29:A:LEU:HB3	1:52:A:PHE:HD1	3	0.3
(1,583)	1:29:A:LEU:HB3	1:52:A:PHE:HD2	3	0.3
(1,523)	1:29:A:LEU:HA	1:52:A:PHE:HD1	3	0.3
(1,523)	1:29:A:LEU:HA	1:52:A:PHE:HD2	3	0.3
(1,516)	1:33:A:ARG:H	1:34:A:ARG:HA	3	0.3
(1,385)	1:54:A:ASN:H	1:55:A:GLU:HA	1	0.3
(1,361)	1:19:A:LEU:HD21	1:52:A:PHE:H	1	0.3
(1,361)	1:19:A:LEU:HD22	1:52:A:PHE:H	1	0.3
(1,361)	1:19:A:LEU:HD23	1:52:A:PHE:H	1	0.3
(1,301)	1:11:A:PHE:HB2	1:12:A:SER:H	3	0.3
(1,300)	1:12:A:SER:H	1:15:A:GLN:HA	3	0.3
(1,244)	1:59:A:ILE:H	1:60:A:LYS:H	1	0.3
(1,38)	1:23:A:PHE:HA	1:51:A:TRP:HH2	2	0.3
(1,34)	1:16:A:LEU:HD11	1:51:A:TRP:HH2	2	0.3
(1,34)	1:16:A:LEU:HD12	1:51:A:TRP:HH2	2	0.3
(1,34)	1:16:A:LEU:HD13	1:51:A:TRP:HH2	2	0.3
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD11	1	0.29
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD12	1	0.29
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD13	1	0.29
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD21	1	0.29
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD22	1	0.29
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD23	1	0.29
(1,1480)	1:19:A:LEU:HG	1:51:A:TRP:HE3	3	0.29
(1,1477)	1:51:A:TRP:HB3	1:52:A:PHE:HA	2	0.29
(1,1367)	1:44:A:ASN:HD21	1:47:A:GLN:H	1	0.29
(1,1308)	1:19:A:LEU:HB2	1:22:A:GLU:HG2	2	0.29
(1,1308)	1:19:A:LEU:HB2	1:22:A:GLU:HG3	2	0.29
(1,1308)	1:19:A:LEU:HB3	1:22:A:GLU:HG2	2	0.29
(1,1308)	1:19:A:LEU:HB3	1:22:A:GLU:HG3	2	0.29
(1,1269)	1:33:A:ARG:HE	1:36:A:GLN:HB3	2	0.29
(1,1252)	1:34:A:ARG:HB3	1:48:A:ILE:HB	3	0.29
(1,1180)	1:38:A:SER:HA	1:43:A:LEU:HG	2	0.29
(1,1042)	1:29:A:LEU:HD11	1:30:A:THR:H	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:29:A:LEU:HD12	1:30:A:THR:H	3	0.29
(1,1042)	1:29:A:LEU:HD13	1:30:A:THR:H	3	0.29
(1,770)	1:52:A:PHE:HA	1:55:A:GLU:HG3	3	0.29
(1,760)	1:24:A:ASN:H	1:51:A:TRP:HH2	3	0.29
(1,753)	1:20:A:LYS:H	1:51:A:TRP:HZ2	3	0.29
(1,426)	1:19:A:LEU:HD21	1:20:A:LYS:H	2	0.29
(1,426)	1:19:A:LEU:HD22	1:20:A:LYS:H	2	0.29
(1,426)	1:19:A:LEU:HD23	1:20:A:LYS:H	2	0.29
(1,317)	1:45:A:GLU:H	1:46:A:ALA:HA	1	0.29
(1,303)	1:12:A:SER:H	1:15:A:GLN:HB3	2	0.29
(1,1831)	1:43:A:LEU:HD11	1:48:A:ILE:HG21	3	0.28
(1,1831)	1:43:A:LEU:HD11	1:48:A:ILE:HG22	3	0.28
(1,1831)	1:43:A:LEU:HD11	1:48:A:ILE:HG23	3	0.28
(1,1831)	1:43:A:LEU:HD12	1:48:A:ILE:HG21	3	0.28
(1,1831)	1:43:A:LEU:HD12	1:48:A:ILE:HG22	3	0.28
(1,1831)	1:43:A:LEU:HD12	1:48:A:ILE:HG23	3	0.28
(1,1831)	1:43:A:LEU:HD13	1:48:A:ILE:HG21	3	0.28
(1,1831)	1:43:A:LEU:HD13	1:48:A:ILE:HG22	3	0.28
(1,1831)	1:43:A:LEU:HD13	1:48:A:ILE:HG23	3	0.28
(1,1831)	1:43:A:LEU:HD21	1:48:A:ILE:HG21	3	0.28
(1,1831)	1:43:A:LEU:HD21	1:48:A:ILE:HG22	3	0.28
(1,1831)	1:43:A:LEU:HD21	1:48:A:ILE:HG23	3	0.28
(1,1831)	1:43:A:LEU:HD22	1:48:A:ILE:HG21	3	0.28
(1,1831)	1:43:A:LEU:HD22	1:48:A:ILE:HG22	3	0.28
(1,1831)	1:43:A:LEU:HD22	1:48:A:ILE:HG23	3	0.28
(1,1831)	1:43:A:LEU:HD23	1:48:A:ILE:HG21	3	0.28
(1,1831)	1:43:A:LEU:HD23	1:48:A:ILE:HG22	3	0.28
(1,1831)	1:43:A:LEU:HD23	1:48:A:ILE:HG23	3	0.28
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD11	2	0.28
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD12	2	0.28
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD13	2	0.28
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD21	2	0.28
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD22	2	0.28
(1,1794)	1:38:A:SER:HA	1:41:A:LEU:HD23	2	0.28
(1,1748)	1:32:A:ARG:HA	1:32:A:ARG:HD2	3	0.28
(1,1748)	1:32:A:ARG:HA	1:32:A:ARG:HD3	3	0.28
(1,1731)	1:29:A:LEU:HD11	1:49:A:LYS:HB2	1	0.28
(1,1731)	1:29:A:LEU:HD12	1:49:A:LYS:HB2	1	0.28
(1,1731)	1:29:A:LEU:HD13	1:49:A:LYS:HB2	1	0.28
(1,1731)	1:29:A:LEU:HD21	1:49:A:LYS:HB2	1	0.28
(1,1731)	1:29:A:LEU:HD22	1:49:A:LYS:HB2	1	0.28
(1,1731)	1:29:A:LEU:HD23	1:49:A:LYS:HB2	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1717)	1:29:A:LEU:HD11	1:34:A:ARG:HB2	2	0.28
(1,1717)	1:29:A:LEU:HD12	1:34:A:ARG:HB2	2	0.28
(1,1717)	1:29:A:LEU:HD13	1:34:A:ARG:HB2	2	0.28
(1,1717)	1:29:A:LEU:HD21	1:34:A:ARG:HB2	2	0.28
(1,1717)	1:29:A:LEU:HD22	1:34:A:ARG:HB2	2	0.28
(1,1717)	1:29:A:LEU:HD23	1:34:A:ARG:HB2	2	0.28
(1,1717)	1:29:A:LEU:HD11	1:34:A:ARG:HB3	2	0.28
(1,1717)	1:29:A:LEU:HD12	1:34:A:ARG:HB3	2	0.28
(1,1717)	1:29:A:LEU:HD13	1:34:A:ARG:HB3	2	0.28
(1,1717)	1:29:A:LEU:HD21	1:34:A:ARG:HB3	2	0.28
(1,1717)	1:29:A:LEU:HD22	1:34:A:ARG:HB3	2	0.28
(1,1717)	1:29:A:LEU:HD23	1:34:A:ARG:HB3	2	0.28
(1,1669)	1:24:A:ASN:HD21	1:25:A:GLU:HA	3	0.28
(1,1669)	1:24:A:ASN:HD22	1:25:A:GLU:HA	3	0.28
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD11	3	0.28
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD12	3	0.28
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD13	3	0.28
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD21	3	0.28
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD22	3	0.28
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD23	3	0.28
(1,1451)	1:54:A:ASN:H	1:57:A:ALA:H	2	0.28
(1,1439)	1:7:A:PRO:HD2	1:8:A:ARG:H	1	0.28
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD11	1	0.28
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD12	1	0.28
(1,1243)	1:34:A:ARG:HB3	1:48:A:ILE:HD13	1	0.28
(1,1122)	1:50:A:ILE:HG21	1:54:A:ASN:HB2	2	0.28
(1,1122)	1:50:A:ILE:HG22	1:54:A:ASN:HB2	2	0.28
(1,1122)	1:50:A:ILE:HG23	1:54:A:ASN:HB2	2	0.28
(1,1061)	1:12:A:SER:H	1:43:A:LEU:HD11	2	0.28
(1,1061)	1:12:A:SER:H	1:43:A:LEU:HD12	2	0.28
(1,1061)	1:12:A:SER:H	1:43:A:LEU:HD13	2	0.28
(1,1050)	1:38:A:SER:HA	1:43:A:LEU:HD11	3	0.28
(1,1050)	1:38:A:SER:HA	1:43:A:LEU:HD12	3	0.28
(1,1050)	1:38:A:SER:HA	1:43:A:LEU:HD13	3	0.28
(1,905)	1:9:A:THR:HG21	1:51:A:TRP:HB2	2	0.28
(1,905)	1:9:A:THR:HG22	1:51:A:TRP:HB2	2	0.28
(1,905)	1:9:A:THR:HG23	1:51:A:TRP:HB2	2	0.28
(1,775)	1:55:A:GLU:HA	1:58:A:LYS:HG2	3	0.28
(1,602)	1:16:A:LEU:HB3	1:51:A:TRP:HZ2	2	0.28
(1,341)	1:12:A:SER:HB3	1:14:A:GLU:H	3	0.28
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB1	3	0.28
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB2	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB3	3	0.28
(1,293)	1:11:A:PHE:HE1	1:51:A:TRP:HE1	2	0.28
(1,293)	1:11:A:PHE:HE2	1:51:A:TRP:HE1	2	0.28
(1,277)	1:10:A:ALA:H	1:11:A:PHE:H	1	0.28
(1,1861)	1:52:A:PHE:HA	1:55:A:GLU:HG2	2	0.27
(1,1861)	1:52:A:PHE:HA	1:55:A:GLU:HG3	2	0.27
(1,1731)	1:29:A:LEU:HD11	1:49:A:LYS:HB2	3	0.27
(1,1731)	1:29:A:LEU:HD12	1:49:A:LYS:HB2	3	0.27
(1,1731)	1:29:A:LEU:HD13	1:49:A:LYS:HB2	3	0.27
(1,1731)	1:29:A:LEU:HD21	1:49:A:LYS:HB2	3	0.27
(1,1731)	1:29:A:LEU:HD22	1:49:A:LYS:HB2	3	0.27
(1,1731)	1:29:A:LEU:HD23	1:49:A:LYS:HB2	3	0.27
(1,1476)	1:51:A:TRP:HB3	1:52:A:PHE:HB2	1	0.27
(1,1421)	1:52:A:PHE:HA	1:55:A:GLU:HA	1	0.27
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD21	2	0.27
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD22	2	0.27
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD23	2	0.27
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD21	2	0.27
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD22	2	0.27
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD23	2	0.27
(1,1054)	1:19:A:LEU:HD21	1:23:A:PHE:HD1	2	0.27
(1,1054)	1:19:A:LEU:HD21	1:23:A:PHE:HD2	2	0.27
(1,1054)	1:19:A:LEU:HD22	1:23:A:PHE:HD1	2	0.27
(1,1054)	1:19:A:LEU:HD22	1:23:A:PHE:HD2	2	0.27
(1,1054)	1:19:A:LEU:HD23	1:23:A:PHE:HD1	2	0.27
(1,1054)	1:19:A:LEU:HD23	1:23:A:PHE:HD2	2	0.27
(1,1008)	1:20:A:LYS:H	1:20:A:LYS:HD2	3	0.27
(1,1008)	1:20:A:LYS:H	1:20:A:LYS:HD3	3	0.27
(1,898)	1:21:A:ARG:HD2	1:22:A:GLU:H	1	0.27
(1,898)	1:21:A:ARG:HD3	1:22:A:GLU:H	1	0.27
(1,680)	1:23:A:PHE:HE1	1:28:A:TYR:HA	2	0.27
(1,680)	1:23:A:PHE:HE2	1:28:A:TYR:HA	2	0.27
(1,618)	1:16:A:LEU:HA	1:18:A:ARG:H	1	0.27
(1,611)	1:58:A:LYS:HB2	1:59:A:ILE:H	3	0.27
(1,546)	1:24:A:ASN:H	1:24:A:ASN:HD22	1	0.27
(1,544)	1:42:A:GLY:H	1:43:A:LEU:HA	1	0.27
(1,523)	1:29:A:LEU:HA	1:52:A:PHE:HD1	2	0.27
(1,523)	1:29:A:LEU:HA	1:52:A:PHE:HD2	2	0.27
(1,508)	1:19:A:LEU:HD11	1:52:A:PHE:HD1	2	0.27
(1,508)	1:19:A:LEU:HD11	1:52:A:PHE:HD2	2	0.27
(1,508)	1:19:A:LEU:HD12	1:52:A:PHE:HD1	2	0.27
(1,508)	1:19:A:LEU:HD12	1:52:A:PHE:HD2	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:19:A:LEU:HD13	1:52:A:PHE:HD1	2	0.27
(1,508)	1:19:A:LEU:HD13	1:52:A:PHE:HD2	2	0.27
(1,505)	1:44:A:ASN:HA	1:47:A:GLN:H	1	0.27
(1,490)	1:9:A:THR:HG21	1:11:A:PHE:H	3	0.27
(1,490)	1:9:A:THR:HG22	1:11:A:PHE:H	3	0.27
(1,490)	1:9:A:THR:HG23	1:11:A:PHE:H	3	0.27
(1,16)	1:12:A:SER:H	1:15:A:GLN:H	2	0.27
(1,1894)	1:58:A:LYS:HA	1:58:A:LYS:HE2	1	0.26
(1,1894)	1:58:A:LYS:HA	1:58:A:LYS:HE3	1	0.26
(1,1790)	1:37:A:LEU:HD11	1:51:A:TRP:HB3	2	0.26
(1,1790)	1:37:A:LEU:HD12	1:51:A:TRP:HB3	2	0.26
(1,1790)	1:37:A:LEU:HD13	1:51:A:TRP:HB3	2	0.26
(1,1790)	1:37:A:LEU:HD21	1:51:A:TRP:HB3	2	0.26
(1,1790)	1:37:A:LEU:HD22	1:51:A:TRP:HB3	2	0.26
(1,1790)	1:37:A:LEU:HD23	1:51:A:TRP:HB3	2	0.26
(1,1788)	1:37:A:LEU:HD11	1:40:A:GLU:HG2	1	0.26
(1,1788)	1:37:A:LEU:HD11	1:40:A:GLU:HG3	1	0.26
(1,1788)	1:37:A:LEU:HD12	1:40:A:GLU:HG2	1	0.26
(1,1788)	1:37:A:LEU:HD12	1:40:A:GLU:HG3	1	0.26
(1,1788)	1:37:A:LEU:HD13	1:40:A:GLU:HG2	1	0.26
(1,1788)	1:37:A:LEU:HD13	1:40:A:GLU:HG3	1	0.26
(1,1788)	1:37:A:LEU:HD21	1:40:A:GLU:HG2	1	0.26
(1,1788)	1:37:A:LEU:HD21	1:40:A:GLU:HG3	1	0.26
(1,1788)	1:37:A:LEU:HD22	1:40:A:GLU:HG2	1	0.26
(1,1788)	1:37:A:LEU:HD22	1:40:A:GLU:HG3	1	0.26
(1,1788)	1:37:A:LEU:HD23	1:40:A:GLU:HG2	1	0.26
(1,1788)	1:37:A:LEU:HD23	1:40:A:GLU:HG3	1	0.26
(1,1666)	1:24:A:ASN:HB2	1:25:A:GLU:H	1	0.26
(1,1666)	1:24:A:ASN:HB3	1:25:A:GLU:H	1	0.26
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD11	3	0.26
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD12	3	0.26
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD13	3	0.26
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD21	3	0.26
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD22	3	0.26
(1,1627)	1:19:A:LEU:HD21	1:43:A:LEU:HD23	3	0.26
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD11	3	0.26
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD12	3	0.26
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD13	3	0.26
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD21	3	0.26
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD22	3	0.26
(1,1627)	1:19:A:LEU:HD22	1:43:A:LEU:HD23	3	0.26
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD11	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD12	3	0.26
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD13	3	0.26
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD21	3	0.26
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD22	3	0.26
(1,1627)	1:19:A:LEU:HD23	1:43:A:LEU:HD23	3	0.26
(1,1431)	1:45:A:GLU:HB3	1:47:A:GLN:H	1	0.26
(1,1406)	1:51:A:TRP:HB2	1:52:A:PHE:HA	1	0.26
(1,1319)	1:20:A:LYS:HA	1:23:A:PHE:HB2	3	0.26
(1,1301)	1:25:A:GLU:HG2	1:26:A:ASN:H	2	0.26
(1,1300)	1:35:A:GLN:HE22	1:36:A:GLN:HB2	2	0.26
(1,1131)	1:34:A:ARG:HA	1:48:A:ILE:HG12	3	0.26
(1,1131)	1:34:A:ARG:HA	1:48:A:ILE:HG13	3	0.26
(1,1099)	1:11:A:PHE:HD1	1:19:A:LEU:HB2	3	0.26
(1,1099)	1:11:A:PHE:HD1	1:19:A:LEU:HB3	3	0.26
(1,1099)	1:11:A:PHE:HD2	1:19:A:LEU:HB2	3	0.26
(1,1099)	1:11:A:PHE:HD2	1:19:A:LEU:HB3	3	0.26
(1,1072)	1:41:A:LEU:HB2	1:43:A:LEU:HD21	3	0.26
(1,1072)	1:41:A:LEU:HB2	1:43:A:LEU:HD22	3	0.26
(1,1072)	1:41:A:LEU:HB2	1:43:A:LEU:HD23	3	0.26
(1,1064)	1:19:A:LEU:HD21	1:22:A:GLU:HB3	3	0.26
(1,1064)	1:19:A:LEU:HD22	1:22:A:GLU:HB3	3	0.26
(1,1064)	1:19:A:LEU:HD23	1:22:A:GLU:HB3	3	0.26
(1,1054)	1:19:A:LEU:HD21	1:23:A:PHE:HD1	1	0.26
(1,1054)	1:19:A:LEU:HD21	1:23:A:PHE:HD2	1	0.26
(1,1054)	1:19:A:LEU:HD22	1:23:A:PHE:HD1	1	0.26
(1,1054)	1:19:A:LEU:HD22	1:23:A:PHE:HD2	1	0.26
(1,1054)	1:19:A:LEU:HD23	1:23:A:PHE:HD1	1	0.26
(1,1054)	1:19:A:LEU:HD23	1:23:A:PHE:HD2	1	0.26
(1,1042)	1:29:A:LEU:HD11	1:30:A:THR:H	1	0.26
(1,1042)	1:29:A:LEU:HD12	1:30:A:THR:H	1	0.26
(1,1042)	1:29:A:LEU:HD13	1:30:A:THR:H	1	0.26
(1,1009)	1:5:A:LYS:H	1:5:A:LYS:HD2	3	0.26
(1,1009)	1:5:A:LYS:H	1:5:A:LYS:HD3	3	0.26
(1,899)	1:29:A:LEU:H	1:52:A:PHE:HB2	3	0.26
(1,722)	1:23:A:PHE:HE1	1:27:A:ARG:HB2	2	0.26
(1,722)	1:23:A:PHE:HE2	1:27:A:ARG:HB2	2	0.26
(1,720)	1:23:A:PHE:HD1	1:27:A:ARG:HB2	2	0.26
(1,720)	1:23:A:PHE:HD2	1:27:A:ARG:HB2	2	0.26
(1,666)	1:23:A:PHE:HD1	1:52:A:PHE:HB2	1	0.26
(1,666)	1:23:A:PHE:HD2	1:52:A:PHE:HB2	1	0.26
(1,666)	1:23:A:PHE:HD1	1:52:A:PHE:HB2	2	0.26
(1,666)	1:23:A:PHE:HD2	1:52:A:PHE:HB2	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:23:A:PHE:HB3	1:51:A:TRP:HE3	2	0.26
(1,622)	1:11:A:PHE:HZ	1:48:A:ILE:HA	3	0.26
(1,394)	1:44:A:ASN:HD21	1:46:A:ALA:H	3	0.26
(1,332)	1:23:A:PHE:H	1:51:A:TRP:HZ3	3	0.26
(1,314)	1:45:A:GLU:H	1:48:A:ILE:HB	2	0.26
(1,251)	1:32:A:ARG:H	1:33:A:ARG:HB2	1	0.26
(1,251)	1:32:A:ARG:H	1:33:A:ARG:HB3	1	0.26
(1,247)	1:34:A:ARG:HG2	1:49:A:LYS:H	3	0.26
(1,247)	1:34:A:ARG:HG3	1:49:A:LYS:H	3	0.26
(1,165)	1:11:A:PHE:HD1	1:16:A:LEU:HA	2	0.26
(1,165)	1:11:A:PHE:HD2	1:16:A:LEU:HA	2	0.26
(1,155)	1:35:A:GLN:HA	1:35:A:GLN:HE21	3	0.26
(1,1609)	1:18:A:ARG:HD2	1:22:A:GLU:H	3	0.25
(1,1609)	1:18:A:ARG:HD3	1:22:A:GLU:H	3	0.25
(1,1394)	1:11:A:PHE:HD1	1:16:A:LEU:HB3	2	0.25
(1,1394)	1:11:A:PHE:HD2	1:16:A:LEU:HB3	2	0.25
(1,1343)	1:22:A:GLU:HG2	1:37:A:LEU:H	3	0.25
(1,1343)	1:22:A:GLU:HG3	1:37:A:LEU:H	3	0.25
(1,1295)	1:44:A:ASN:HA	1:45:A:GLU:HG2	1	0.25
(1,1226)	1:57:A:ALA:HB1	1:59:A:ILE:H	1	0.25
(1,1226)	1:57:A:ALA:HB2	1:59:A:ILE:H	1	0.25
(1,1226)	1:57:A:ALA:HB3	1:59:A:ILE:H	1	0.25
(1,1186)	1:11:A:PHE:HE1	1:43:A:LEU:HG	1	0.25
(1,1186)	1:11:A:PHE:HE2	1:43:A:LEU:HG	1	0.25
(1,1104)	1:39:A:SER:H	1:48:A:ILE:HD11	1	0.25
(1,1104)	1:39:A:SER:H	1:48:A:ILE:HD12	1	0.25
(1,1104)	1:39:A:SER:H	1:48:A:ILE:HD13	1	0.25
(1,1038)	1:29:A:LEU:HD11	1:33:A:ARG:HA	3	0.25
(1,1038)	1:29:A:LEU:HD12	1:33:A:ARG:HA	3	0.25
(1,1038)	1:29:A:LEU:HD13	1:33:A:ARG:HA	3	0.25
(1,1024)	1:15:A:GLN:H	1:15:A:GLN:HG2	3	0.25
(1,748)	1:44:A:ASN:HD22	1:47:A:GLN:HE21	3	0.25
(1,689)	1:23:A:PHE:HE1	1:27:A:ARG:H	1	0.25
(1,689)	1:23:A:PHE:HE2	1:27:A:ARG:H	1	0.25
(1,654)	1:48:A:ILE:HG21	1:51:A:TRP:HE3	3	0.25
(1,654)	1:48:A:ILE:HG22	1:51:A:TRP:HE3	3	0.25
(1,654)	1:48:A:ILE:HG23	1:51:A:TRP:HE3	3	0.25
(1,644)	1:19:A:LEU:HD11	1:51:A:TRP:HZ2	3	0.25
(1,644)	1:19:A:LEU:HD12	1:51:A:TRP:HZ2	3	0.25
(1,644)	1:19:A:LEU:HD13	1:51:A:TRP:HZ2	3	0.25
(1,626)	1:11:A:PHE:HE1	1:47:A:GLN:HA	2	0.25
(1,626)	1:11:A:PHE:HE2	1:47:A:GLN:HA	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:29:A:LEU:HA	1:52:A:PHE:HE1	3	0.25
(1,594)	1:29:A:LEU:HA	1:52:A:PHE:HE2	3	0.25
(1,439)	1:27:A:ARG:H	1:28:A:TYR:HE1	1	0.25
(1,439)	1:27:A:ARG:H	1:28:A:TYR:HE2	1	0.25
(1,331)	1:23:A:PHE:H	1:24:A:ASN:HA	1	0.25
(1,209)	1:57:A:ALA:HB1	1:58:A:LYS:HA	1	0.25
(1,209)	1:57:A:ALA:HB2	1:58:A:LYS:HA	1	0.25
(1,209)	1:57:A:ALA:HB3	1:58:A:LYS:HA	1	0.25
(1,66)	1:23:A:PHE:HB3	1:52:A:PHE:HE1	1	0.25
(1,66)	1:23:A:PHE:HB3	1:52:A:PHE:HE2	1	0.25
(1,1894)	1:58:A:LYS:HA	1:58:A:LYS:HE2	3	0.24
(1,1894)	1:58:A:LYS:HA	1:58:A:LYS:HE3	3	0.24
(1,1851)	1:50:A:ILE:HD11	1:53:A:GLN:HE21	2	0.24
(1,1851)	1:50:A:ILE:HD11	1:53:A:GLN:HE22	2	0.24
(1,1851)	1:50:A:ILE:HD12	1:53:A:GLN:HE21	2	0.24
(1,1851)	1:50:A:ILE:HD12	1:53:A:GLN:HE22	2	0.24
(1,1851)	1:50:A:ILE:HD13	1:53:A:GLN:HE21	2	0.24
(1,1851)	1:50:A:ILE:HD13	1:53:A:GLN:HE22	2	0.24
(1,1818)	1:41:A:LEU:HD11	1:43:A:LEU:HG	3	0.24
(1,1818)	1:41:A:LEU:HD12	1:43:A:LEU:HG	3	0.24
(1,1818)	1:41:A:LEU:HD13	1:43:A:LEU:HG	3	0.24
(1,1818)	1:41:A:LEU:HD21	1:43:A:LEU:HG	3	0.24
(1,1818)	1:41:A:LEU:HD22	1:43:A:LEU:HG	3	0.24
(1,1818)	1:41:A:LEU:HD23	1:43:A:LEU:HG	3	0.24
(1,1662)	1:24:A:ASN:H	1:24:A:ASN:HD21	1	0.24
(1,1662)	1:24:A:ASN:H	1:24:A:ASN:HD22	1	0.24
(1,1651)	1:23:A:PHE:HD1	1:59:A:ILE:HG12	1	0.24
(1,1651)	1:23:A:PHE:HD1	1:59:A:ILE:HG13	1	0.24
(1,1651)	1:23:A:PHE:HD2	1:59:A:ILE:HG12	1	0.24
(1,1651)	1:23:A:PHE:HD2	1:59:A:ILE:HG13	1	0.24
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD11	3	0.24
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD12	3	0.24
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD13	3	0.24
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD21	3	0.24
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD22	3	0.24
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD23	3	0.24
(1,1476)	1:51:A:TRP:HB3	1:52:A:PHE:HB2	2	0.24
(1,1357)	1:16:A:LEU:HA	1:20:A:LYS:HB2	1	0.24
(1,1235)	1:45:A:GLU:H	1:46:A:ALA:HB1	1	0.24
(1,1235)	1:45:A:GLU:H	1:46:A:ALA:HB2	1	0.24
(1,1235)	1:45:A:GLU:H	1:46:A:ALA:HB3	1	0.24
(1,1213)	1:28:A:TYR:HA	1:29:A:LEU:HB3	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB1	1	0.24
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB2	1	0.24
(1,1210)	1:13:A:SER:HA	1:17:A:ALA:HB3	1	0.24
(1,1174)	1:19:A:LEU:HD21	1:41:A:LEU:HG	1	0.24
(1,1174)	1:19:A:LEU:HD22	1:41:A:LEU:HG	1	0.24
(1,1174)	1:19:A:LEU:HD23	1:41:A:LEU:HG	1	0.24
(1,1160)	1:38:A:SER:H	1:48:A:ILE:HG12	3	0.24
(1,1160)	1:38:A:SER:H	1:48:A:ILE:HG13	3	0.24
(1,1110)	1:19:A:LEU:HD21	1:41:A:LEU:HD21	1	0.24
(1,1110)	1:19:A:LEU:HD21	1:41:A:LEU:HD22	1	0.24
(1,1110)	1:19:A:LEU:HD21	1:41:A:LEU:HD23	1	0.24
(1,1110)	1:19:A:LEU:HD22	1:41:A:LEU:HD21	1	0.24
(1,1110)	1:19:A:LEU:HD22	1:41:A:LEU:HD22	1	0.24
(1,1110)	1:19:A:LEU:HD22	1:41:A:LEU:HD23	1	0.24
(1,1110)	1:19:A:LEU:HD23	1:41:A:LEU:HD21	1	0.24
(1,1110)	1:19:A:LEU:HD23	1:41:A:LEU:HD22	1	0.24
(1,1110)	1:19:A:LEU:HD23	1:41:A:LEU:HD23	1	0.24
(1,1038)	1:29:A:LEU:HD11	1:33:A:ARG:HA	1	0.24
(1,1038)	1:29:A:LEU:HD12	1:33:A:ARG:HA	1	0.24
(1,1038)	1:29:A:LEU:HD13	1:33:A:ARG:HA	1	0.24
(1,1038)	1:29:A:LEU:HD11	1:33:A:ARG:HA	2	0.24
(1,1038)	1:29:A:LEU:HD12	1:33:A:ARG:HA	2	0.24
(1,1038)	1:29:A:LEU:HD13	1:33:A:ARG:HA	2	0.24
(1,750)	1:11:A:PHE:HD1	1:15:A:GLN:HE22	1	0.24
(1,750)	1:11:A:PHE:HD2	1:15:A:GLN:HE22	1	0.24
(1,733)	1:23:A:PHE:HD1	1:56:A:ARG:HA	3	0.24
(1,733)	1:23:A:PHE:HD2	1:56:A:ARG:HA	3	0.24
(1,697)	1:11:A:PHE:HZ	1:51:A:TRP:HE1	2	0.24
(1,583)	1:29:A:LEU:HB3	1:52:A:PHE:HD1	1	0.24
(1,583)	1:29:A:LEU:HB3	1:52:A:PHE:HD2	1	0.24
(1,399)	1:8:A:ARG:H	1:9:A:THR:HG21	2	0.24
(1,399)	1:8:A:ARG:H	1:9:A:THR:HG22	2	0.24
(1,399)	1:8:A:ARG:H	1:9:A:THR:HG23	2	0.24
(1,247)	1:34:A:ARG:HG2	1:49:A:LYS:H	1	0.24
(1,247)	1:34:A:ARG:HG3	1:49:A:LYS:H	1	0.24
(1,236)	1:59:A:ILE:H	1:59:A:ILE:HB	3	0.24
(1,29)	1:19:A:LEU:HD11	1:51:A:TRP:HH2	3	0.24
(1,29)	1:19:A:LEU:HD12	1:51:A:TRP:HH2	3	0.24
(1,29)	1:19:A:LEU:HD13	1:51:A:TRP:HH2	3	0.24
(1,25)	1:15:A:GLN:H	1:17:A:ALA:H	2	0.24
(1,1740)	1:30:A:THR:HA	1:31:A:GLU:HG2	1	0.23
(1,1740)	1:30:A:THR:HA	1:31:A:GLU:HG3	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1585)	1:16:A:LEU:HD11	1:18:A:ARG:H	2	0.23
(1,1585)	1:16:A:LEU:HD12	1:18:A:ARG:H	2	0.23
(1,1585)	1:16:A:LEU:HD13	1:18:A:ARG:H	2	0.23
(1,1585)	1:16:A:LEU:HD21	1:18:A:ARG:H	2	0.23
(1,1585)	1:16:A:LEU:HD22	1:18:A:ARG:H	2	0.23
(1,1585)	1:16:A:LEU:HD23	1:18:A:ARG:H	2	0.23
(1,1540)	1:12:A:SER:HB2	1:15:A:GLN:H	3	0.23
(1,1540)	1:12:A:SER:HB3	1:15:A:GLN:H	3	0.23
(1,1482)	1:11:A:PHE:HB2	1:16:A:LEU:HB2	2	0.23
(1,1480)	1:19:A:LEU:HG	1:51:A:TRP:HE3	1	0.23
(1,1431)	1:45:A:GLU:HB3	1:47:A:GLN:H	2	0.23
(1,1365)	1:38:A:SER:H	1:42:A:GLY:H	2	0.23
(1,1256)	1:34:A:ARG:HA	1:48:A:ILE:HB	2	0.23
(1,1142)	1:9:A:THR:HG21	1:10:A:ALA:HA	2	0.23
(1,1142)	1:9:A:THR:HG22	1:10:A:ALA:HA	2	0.23
(1,1142)	1:9:A:THR:HG23	1:10:A:ALA:HA	2	0.23
(1,1141)	1:50:A:ILE:HG21	1:54:A:ASN:HA	1	0.23
(1,1141)	1:50:A:ILE:HG22	1:54:A:ASN:HA	1	0.23
(1,1141)	1:50:A:ILE:HG23	1:54:A:ASN:HA	1	0.23
(1,1105)	1:41:A:LEU:HD21	1:42:A:GLY:H	1	0.23
(1,1105)	1:41:A:LEU:HD22	1:42:A:GLY:H	1	0.23
(1,1105)	1:41:A:LEU:HD23	1:42:A:GLY:H	1	0.23
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD21	1	0.23
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD22	1	0.23
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD23	1	0.23
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD21	1	0.23
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD22	1	0.23
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD23	1	0.23
(1,1049)	1:19:A:LEU:HD21	1:37:A:LEU:HA	2	0.23
(1,1049)	1:19:A:LEU:HD22	1:37:A:LEU:HA	2	0.23
(1,1049)	1:19:A:LEU:HD23	1:37:A:LEU:HA	2	0.23
(1,1005)	1:60:A:LYS:H	1:60:A:LYS:HD2	1	0.23
(1,1005)	1:60:A:LYS:H	1:60:A:LYS:HD3	1	0.23
(1,953)	1:53:A:GLN:H	1:53:A:GLN:HB3	1	0.23
(1,733)	1:23:A:PHE:HD1	1:56:A:ARG:HA	1	0.23
(1,733)	1:23:A:PHE:HD2	1:56:A:ARG:HA	1	0.23
(1,692)	1:58:A:LYS:H	1:60:A:LYS:H	1	0.23
(1,650)	1:23:A:PHE:HE1	1:55:A:GLU:HB2	1	0.23
(1,650)	1:23:A:PHE:HE2	1:55:A:GLU:HB2	1	0.23
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD11	1	0.23
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD12	1	0.23
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD13	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:22:A:GLU:HA	1:52:A:PHE:HE1	2	0.23
(1,563)	1:22:A:GLU:HA	1:52:A:PHE:HE2	2	0.23
(1,563)	1:22:A:GLU:HA	1:52:A:PHE:HE1	3	0.23
(1,563)	1:22:A:GLU:HA	1:52:A:PHE:HE2	3	0.23
(1,517)	1:15:A:GLN:H	1:16:A:LEU:HA	2	0.23
(1,464)	1:24:A:ASN:H	1:26:A:ASN:H	1	0.23
(1,407)	1:18:A:ARG:HE	1:41:A:LEU:HD11	1	0.23
(1,407)	1:18:A:ARG:HE	1:41:A:LEU:HD12	1	0.23
(1,407)	1:18:A:ARG:HE	1:41:A:LEU:HD13	1	0.23
(1,372)	1:44:A:ASN:H	1:46:A:ALA:H	2	0.23
(1,333)	1:23:A:PHE:H	1:51:A:TRP:HH2	3	0.23
(1,262)	1:15:A:GLN:H	1:15:A:GLN:HE21	1	0.23
(1,108)	1:10:A:ALA:H	1:47:A:GLN:HE22	2	0.23
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD11	3	0.22
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD12	3	0.22
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD13	3	0.22
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD21	3	0.22
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD22	3	0.22
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD23	3	0.22
(1,1802)	1:38:A:SER:HB2	1:48:A:ILE:HG12	2	0.22
(1,1802)	1:38:A:SER:HB2	1:48:A:ILE:HG13	2	0.22
(1,1802)	1:38:A:SER:HB3	1:48:A:ILE:HG12	2	0.22
(1,1802)	1:38:A:SER:HB3	1:48:A:ILE:HG13	2	0.22
(1,1687)	1:26:A:ASN:HD21	1:27:A:ARG:H	2	0.22
(1,1687)	1:26:A:ASN:HD22	1:27:A:ARG:H	2	0.22
(1,1613)	1:18:A:ARG:HE	1:37:A:LEU:HD11	1	0.22
(1,1613)	1:18:A:ARG:HE	1:37:A:LEU:HD12	1	0.22
(1,1613)	1:18:A:ARG:HE	1:37:A:LEU:HD13	1	0.22
(1,1613)	1:18:A:ARG:HE	1:37:A:LEU:HD21	1	0.22
(1,1613)	1:18:A:ARG:HE	1:37:A:LEU:HD22	1	0.22
(1,1613)	1:18:A:ARG:HE	1:37:A:LEU:HD23	1	0.22
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD11	1	0.22
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD12	1	0.22
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD13	1	0.22
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD21	1	0.22
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD22	1	0.22
(1,1562)	1:15:A:GLN:H	1:41:A:LEU:HD23	1	0.22
(1,1540)	1:12:A:SER:HB2	1:15:A:GLN:H	1	0.22
(1,1540)	1:12:A:SER:HB3	1:15:A:GLN:H	1	0.22
(1,1431)	1:45:A:GLU:HB3	1:47:A:GLN:H	3	0.22
(1,1411)	1:26:A:ASN:HA	1:27:A:ARG:HG2	1	0.22
(1,1404)	1:34:A:ARG:HD3	1:45:A:GLU:HA	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:49:A:LYS:HB2	1:50:A:ILE:HA	2	0.22
(1,1331)	1:11:A:PHE:HE1	1:47:A:GLN:HG3	3	0.22
(1,1331)	1:11:A:PHE:HE2	1:47:A:GLN:HG3	3	0.22
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD11	2	0.22
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD12	2	0.22
(1,1060)	1:41:A:LEU:H	1:43:A:LEU:HD13	2	0.22
(1,1047)	1:29:A:LEU:HD21	1:52:A:PHE:HB2	1	0.22
(1,1047)	1:29:A:LEU:HD22	1:52:A:PHE:HB2	1	0.22
(1,1047)	1:29:A:LEU:HD23	1:52:A:PHE:HB2	1	0.22
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD11	2	0.22
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD12	2	0.22
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD13	2	0.22
(1,942)	1:32:A:ARG:HA	1:32:A:ARG:HG3	3	0.22
(1,817)	1:11:A:PHE:HD1	1:15:A:GLN:HA	3	0.22
(1,817)	1:11:A:PHE:HD2	1:15:A:GLN:HA	3	0.22
(1,720)	1:23:A:PHE:HD1	1:27:A:ARG:HB2	3	0.22
(1,720)	1:23:A:PHE:HD2	1:27:A:ARG:HB2	3	0.22
(1,674)	1:23:A:PHE:HE1	1:56:A:ARG:HA	2	0.22
(1,674)	1:23:A:PHE:HE2	1:56:A:ARG:HA	2	0.22
(1,629)	1:21:A:ARG:H	1:51:A:TRP:HH2	1	0.22
(1,626)	1:11:A:PHE:HE1	1:47:A:GLN:HA	3	0.22
(1,626)	1:11:A:PHE:HE2	1:47:A:GLN:HA	3	0.22
(1,575)	1:29:A:LEU:HG	1:30:A:THR:H	2	0.22
(1,539)	1:32:A:ARG:HB3	1:33:A:ARG:H	1	0.22
(1,488)	1:29:A:LEU:HB3	1:34:A:ARG:HE	2	0.22
(1,410)	1:19:A:LEU:HD11	1:20:A:LYS:H	3	0.22
(1,410)	1:19:A:LEU:HD12	1:20:A:LYS:H	3	0.22
(1,410)	1:19:A:LEU:HD13	1:20:A:LYS:H	3	0.22
(1,341)	1:12:A:SER:HB3	1:14:A:GLU:H	1	0.22
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB1	2	0.22
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB2	2	0.22
(1,310)	1:44:A:ASN:H	1:46:A:ALA:HB3	2	0.22
(1,269)	1:11:A:PHE:H	1:11:A:PHE:HE1	2	0.22
(1,269)	1:11:A:PHE:H	1:11:A:PHE:HE2	2	0.22
(1,189)	1:44:A:ASN:HA	1:44:A:ASN:HD21	1	0.22
(1,55)	1:39:A:SER:H	1:39:A:SER:HB2	2	0.22
(1,55)	1:39:A:SER:H	1:39:A:SER:HB3	2	0.22
(1,35)	1:20:A:LYS:HG2	1:51:A:TRP:HH2	1	0.22
(1,35)	1:20:A:LYS:HG3	1:51:A:TRP:HH2	1	0.22
(1,20)	1:15:A:GLN:HA	1:15:A:GLN:HE21	1	0.22
(1,16)	1:12:A:SER:H	1:15:A:GLN:H	3	0.22
(1,1843)	1:49:A:LYS:HG2	1:50:A:ILE:HA	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1843)	1:49:A:LYS:HG3	1:50:A:ILE:HA	1	0.21
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD11	2	0.21
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD12	2	0.21
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD13	2	0.21
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD21	2	0.21
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD22	2	0.21
(1,1782)	1:37:A:LEU:HA	1:43:A:LEU:HD23	2	0.21
(1,1738)	1:29:A:LEU:HD11	1:53:A:GLN:H	3	0.21
(1,1738)	1:29:A:LEU:HD12	1:53:A:GLN:H	3	0.21
(1,1738)	1:29:A:LEU:HD13	1:53:A:GLN:H	3	0.21
(1,1738)	1:29:A:LEU:HD21	1:53:A:GLN:H	3	0.21
(1,1738)	1:29:A:LEU:HD22	1:53:A:GLN:H	3	0.21
(1,1738)	1:29:A:LEU:HD23	1:53:A:GLN:H	3	0.21
(1,1539)	1:12:A:SER:HB2	1:14:A:GLU:HB2	2	0.21
(1,1539)	1:12:A:SER:HB3	1:14:A:GLU:HB2	2	0.21
(1,1539)	1:12:A:SER:HB2	1:14:A:GLU:HB3	2	0.21
(1,1539)	1:12:A:SER:HB3	1:14:A:GLU:HB3	2	0.21
(1,1497)	1:6:A:ARG:HD2	1:7:A:PRO:HD2	3	0.21
(1,1497)	1:6:A:ARG:HD2	1:7:A:PRO:HD3	3	0.21
(1,1497)	1:6:A:ARG:HD3	1:7:A:PRO:HD2	3	0.21
(1,1497)	1:6:A:ARG:HD3	1:7:A:PRO:HD3	3	0.21
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB1	2	0.21
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB2	2	0.21
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB3	2	0.21
(1,1346)	1:11:A:PHE:HB2	1:19:A:LEU:HD11	3	0.21
(1,1346)	1:11:A:PHE:HB2	1:19:A:LEU:HD12	3	0.21
(1,1346)	1:11:A:PHE:HB2	1:19:A:LEU:HD13	3	0.21
(1,1284)	1:33:A:ARG:HD3	1:36:A:GLN:HB2	1	0.21
(1,1115)	1:34:A:ARG:HG2	1:48:A:ILE:HG12	2	0.21
(1,1115)	1:34:A:ARG:HG2	1:48:A:ILE:HG13	2	0.21
(1,1115)	1:34:A:ARG:HG3	1:48:A:ILE:HG12	2	0.21
(1,1115)	1:34:A:ARG:HG3	1:48:A:ILE:HG13	2	0.21
(1,1104)	1:39:A:SER:H	1:48:A:ILE:HD11	2	0.21
(1,1104)	1:39:A:SER:H	1:48:A:ILE:HD12	2	0.21
(1,1104)	1:39:A:SER:H	1:48:A:ILE:HD13	2	0.21
(1,1049)	1:19:A:LEU:HD21	1:37:A:LEU:HA	1	0.21
(1,1049)	1:19:A:LEU:HD22	1:37:A:LEU:HA	1	0.21
(1,1049)	1:19:A:LEU:HD23	1:37:A:LEU:HA	1	0.21
(1,1048)	1:19:A:LEU:HD21	1:48:A:ILE:HA	1	0.21
(1,1048)	1:19:A:LEU:HD22	1:48:A:ILE:HA	1	0.21
(1,1048)	1:19:A:LEU:HD23	1:48:A:ILE:HA	1	0.21
(1,942)	1:32:A:ARG:HA	1:32:A:ARG:HG3	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,838)	1:51:A:TRP:H	1:52:A:PHE:HA	3	0.21
(1,791)	1:55:A:GLU:HA	1:58:A:LYS:HA	1	0.21
(1,755)	1:51:A:TRP:HD1	1:52:A:PHE:H	2	0.21
(1,707)	1:29:A:LEU:HD21	1:51:A:TRP:HE3	1	0.21
(1,707)	1:29:A:LEU:HD22	1:51:A:TRP:HE3	1	0.21
(1,707)	1:29:A:LEU:HD23	1:51:A:TRP:HE3	1	0.21
(1,654)	1:48:A:ILE:HG21	1:51:A:TRP:HE3	2	0.21
(1,654)	1:48:A:ILE:HG22	1:51:A:TRP:HE3	2	0.21
(1,654)	1:48:A:ILE:HG23	1:51:A:TRP:HE3	2	0.21
(1,633)	1:33:A:ARG:H	1:35:A:GLN:H	1	0.21
(1,393)	1:18:A:ARG:H	1:20:A:LYS:H	1	0.21
(1,393)	1:18:A:ARG:H	1:20:A:LYS:H	2	0.21
(1,342)	1:44:A:ASN:HA	1:46:A:ALA:H	1	0.21
(1,270)	1:11:A:PHE:HA	1:11:A:PHE:HE1	1	0.21
(1,270)	1:11:A:PHE:HA	1:11:A:PHE:HE2	1	0.21
(1,270)	1:11:A:PHE:HA	1:11:A:PHE:HE1	2	0.21
(1,270)	1:11:A:PHE:HA	1:11:A:PHE:HE2	2	0.21
(1,145)	1:34:A:ARG:HA	1:34:A:ARG:HE	2	0.21
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD11	1	0.2
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD12	1	0.2
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD13	1	0.2
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD21	1	0.2
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD22	1	0.2
(1,1813)	1:41:A:LEU:HB2	1:43:A:LEU:HD23	1	0.2
(1,1810)	1:41:A:LEU:HA	1:41:A:LEU:HD11	1	0.2
(1,1810)	1:41:A:LEU:HA	1:41:A:LEU:HD12	1	0.2
(1,1810)	1:41:A:LEU:HA	1:41:A:LEU:HD13	1	0.2
(1,1810)	1:41:A:LEU:HA	1:41:A:LEU:HD21	1	0.2
(1,1810)	1:41:A:LEU:HA	1:41:A:LEU:HD22	1	0.2
(1,1810)	1:41:A:LEU:HA	1:41:A:LEU:HD23	1	0.2
(1,1642)	1:21:A:ARG:HD2	1:24:A:ASN:HD21	2	0.2
(1,1642)	1:21:A:ARG:HD2	1:24:A:ASN:HD22	2	0.2
(1,1642)	1:21:A:ARG:HD3	1:24:A:ASN:HD21	2	0.2
(1,1642)	1:21:A:ARG:HD3	1:24:A:ASN:HD22	2	0.2
(1,1590)	1:16:A:LEU:HD11	1:20:A:LYS:HA	3	0.2
(1,1590)	1:16:A:LEU:HD12	1:20:A:LYS:HA	3	0.2
(1,1590)	1:16:A:LEU:HD13	1:20:A:LYS:HA	3	0.2
(1,1590)	1:16:A:LEU:HD21	1:20:A:LYS:HA	3	0.2
(1,1590)	1:16:A:LEU:HD22	1:20:A:LYS:HA	3	0.2
(1,1590)	1:16:A:LEU:HD23	1:20:A:LYS:HA	3	0.2
(1,1477)	1:51:A:TRP:HB3	1:52:A:PHE:HA	1	0.2
(1,1458)	1:16:A:LEU:HA	1:51:A:TRP:HH2	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1351)	1:34:A:ARG:HG2	1:49:A:LYS:HE2	2	0.2
(1,1351)	1:34:A:ARG:HG2	1:49:A:LYS:HE3	2	0.2
(1,1351)	1:34:A:ARG:HG3	1:49:A:LYS:HE2	2	0.2
(1,1351)	1:34:A:ARG:HG3	1:49:A:LYS:HE3	2	0.2
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB1	3	0.2
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB2	3	0.2
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB3	3	0.2
(1,1341)	1:56:A:ARG:H	1:56:A:ARG:HD2	3	0.2
(1,1271)	1:20:A:LYS:HB3	1:24:A:ASN:HD21	3	0.2
(1,1269)	1:33:A:ARG:HE	1:36:A:GLN:HB3	3	0.2
(1,1174)	1:19:A:LEU:HD21	1:41:A:LEU:HG	2	0.2
(1,1174)	1:19:A:LEU:HD22	1:41:A:LEU:HG	2	0.2
(1,1174)	1:19:A:LEU:HD23	1:41:A:LEU:HG	2	0.2
(1,1142)	1:9:A:THR:HG21	1:10:A:ALA:HA	1	0.2
(1,1142)	1:9:A:THR:HG22	1:10:A:ALA:HA	1	0.2
(1,1142)	1:9:A:THR:HG23	1:10:A:ALA:HA	1	0.2
(1,1126)	1:48:A:ILE:HG21	1:51:A:TRP:HB2	3	0.2
(1,1126)	1:48:A:ILE:HG22	1:51:A:TRP:HB2	3	0.2
(1,1126)	1:48:A:ILE:HG23	1:51:A:TRP:HB2	3	0.2
(1,1059)	1:55:A:GLU:HB2	1:56:A:ARG:H	2	0.2
(1,1058)	1:29:A:LEU:HD21	1:52:A:PHE:HD1	2	0.2
(1,1058)	1:29:A:LEU:HD21	1:52:A:PHE:HD2	2	0.2
(1,1058)	1:29:A:LEU:HD22	1:52:A:PHE:HD1	2	0.2
(1,1058)	1:29:A:LEU:HD22	1:52:A:PHE:HD2	2	0.2
(1,1058)	1:29:A:LEU:HD23	1:52:A:PHE:HD1	2	0.2
(1,1058)	1:29:A:LEU:HD23	1:52:A:PHE:HD2	2	0.2
(1,899)	1:29:A:LEU:H	1:52:A:PHE:HB2	2	0.2
(1,820)	1:23:A:PHE:HZ	1:55:A:GLU:HA	3	0.2
(1,747)	1:23:A:PHE:HD1	1:51:A:TRP:HH2	2	0.2
(1,747)	1:23:A:PHE:HD2	1:51:A:TRP:HH2	2	0.2
(1,728)	1:16:A:LEU:HA	1:51:A:TRP:HZ2	3	0.2
(1,607)	1:43:A:LEU:HB2	1:47:A:GLN:HE22	2	0.2
(1,607)	1:43:A:LEU:HB3	1:47:A:GLN:HE22	2	0.2
(1,546)	1:24:A:ASN:H	1:24:A:ASN:HD22	3	0.2
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD21	1	0.2
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD22	1	0.2
(1,536)	1:42:A:GLY:H	1:43:A:LEU:HD23	1	0.2
(1,478)	1:45:A:GLU:HA	1:47:A:GLN:H	1	0.2
(1,440)	1:22:A:GLU:H	1:52:A:PHE:HZ	2	0.2
(1,426)	1:19:A:LEU:HD21	1:20:A:LYS:H	1	0.2
(1,426)	1:19:A:LEU:HD22	1:20:A:LYS:H	1	0.2
(1,426)	1:19:A:LEU:HD23	1:20:A:LYS:H	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:18:A:ARG:HE	1:41:A:LEU:HD11	2	0.2
(1,407)	1:18:A:ARG:HE	1:41:A:LEU:HD12	2	0.2
(1,407)	1:18:A:ARG:HE	1:41:A:LEU:HD13	2	0.2
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD11	2	0.2
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD12	2	0.2
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD13	2	0.2
(1,189)	1:44:A:ASN:HA	1:44:A:ASN:HD21	3	0.2
(1,1831)	1:43:A:LEU:HD11	1:48:A:ILE:HG21	1	0.19
(1,1831)	1:43:A:LEU:HD11	1:48:A:ILE:HG22	1	0.19
(1,1831)	1:43:A:LEU:HD11	1:48:A:ILE:HG23	1	0.19
(1,1831)	1:43:A:LEU:HD12	1:48:A:ILE:HG21	1	0.19
(1,1831)	1:43:A:LEU:HD12	1:48:A:ILE:HG22	1	0.19
(1,1831)	1:43:A:LEU:HD12	1:48:A:ILE:HG23	1	0.19
(1,1831)	1:43:A:LEU:HD13	1:48:A:ILE:HG21	1	0.19
(1,1831)	1:43:A:LEU:HD13	1:48:A:ILE:HG22	1	0.19
(1,1831)	1:43:A:LEU:HD13	1:48:A:ILE:HG23	1	0.19
(1,1831)	1:43:A:LEU:HD21	1:48:A:ILE:HG21	1	0.19
(1,1831)	1:43:A:LEU:HD21	1:48:A:ILE:HG22	1	0.19
(1,1831)	1:43:A:LEU:HD21	1:48:A:ILE:HG23	1	0.19
(1,1831)	1:43:A:LEU:HD22	1:48:A:ILE:HG21	1	0.19
(1,1831)	1:43:A:LEU:HD22	1:48:A:ILE:HG22	1	0.19
(1,1831)	1:43:A:LEU:HD22	1:48:A:ILE:HG23	1	0.19
(1,1831)	1:43:A:LEU:HD23	1:48:A:ILE:HG21	1	0.19
(1,1831)	1:43:A:LEU:HD23	1:48:A:ILE:HG22	1	0.19
(1,1831)	1:43:A:LEU:HD23	1:48:A:ILE:HG23	1	0.19
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD11	3	0.19
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD12	3	0.19
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD13	3	0.19
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD21	3	0.19
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD22	3	0.19
(1,1778)	1:37:A:LEU:H	1:41:A:LEU:HD23	3	0.19
(1,1747)	1:32:A:ARG:HA	1:32:A:ARG:HG2	3	0.19
(1,1747)	1:32:A:ARG:HA	1:32:A:ARG:HG3	3	0.19
(1,1614)	1:18:A:ARG:HE	1:41:A:LEU:HD11	1	0.19
(1,1614)	1:18:A:ARG:HE	1:41:A:LEU:HD12	1	0.19
(1,1614)	1:18:A:ARG:HE	1:41:A:LEU:HD13	1	0.19
(1,1614)	1:18:A:ARG:HE	1:41:A:LEU:HD21	1	0.19
(1,1614)	1:18:A:ARG:HE	1:41:A:LEU:HD22	1	0.19
(1,1614)	1:18:A:ARG:HE	1:41:A:LEU:HD23	1	0.19
(1,1597)	1:18:A:ARG:H	1:18:A:ARG:HD2	3	0.19
(1,1597)	1:18:A:ARG:H	1:18:A:ARG:HD3	3	0.19
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD11	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD12	2	0.19
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD13	2	0.19
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD21	2	0.19
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD22	2	0.19
(1,1512)	1:11:A:PHE:HA	1:16:A:LEU:HD23	2	0.19
(1,1425)	1:20:A:LYS:HB3	1:24:A:ASN:HD22	3	0.19
(1,1363)	1:18:A:ARG:H	1:21:A:ARG:H	3	0.19
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB1	1	0.19
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB2	1	0.19
(1,1350)	1:44:A:ASN:HB3	1:46:A:ALA:HB3	1	0.19
(1,1341)	1:56:A:ARG:H	1:56:A:ARG:HD2	1	0.19
(1,1319)	1:20:A:LYS:HA	1:23:A:PHE:HB2	1	0.19
(1,1298)	1:15:A:GLN:HE21	1:41:A:LEU:HB2	3	0.19
(1,1053)	1:23:A:PHE:HD1	1:55:A:GLU:HB2	1	0.19
(1,1053)	1:23:A:PHE:HD2	1:55:A:GLU:HB2	1	0.19
(1,880)	1:22:A:GLU:HG2	1:37:A:LEU:HA	1	0.19
(1,880)	1:22:A:GLU:HG3	1:37:A:LEU:HA	1	0.19
(1,797)	1:38:A:SER:HA	1:45:A:GLU:HA	2	0.19
(1,705)	1:23:A:PHE:HZ	1:55:A:GLU:HB2	1	0.19
(1,694)	1:23:A:PHE:HE1	1:28:A:TYR:H	1	0.19
(1,694)	1:23:A:PHE:HE2	1:28:A:TYR:H	1	0.19
(1,625)	1:19:A:LEU:HA	1:52:A:PHE:HE1	2	0.19
(1,625)	1:19:A:LEU:HA	1:52:A:PHE:HE2	2	0.19
(1,410)	1:19:A:LEU:HD11	1:20:A:LYS:H	1	0.19
(1,410)	1:19:A:LEU:HD12	1:20:A:LYS:H	1	0.19
(1,410)	1:19:A:LEU:HD13	1:20:A:LYS:H	1	0.19
(1,387)	1:38:A:SER:HA	1:40:A:GLU:H	3	0.19
(1,372)	1:44:A:ASN:H	1:46:A:ALA:H	3	0.19
(1,322)	1:44:A:ASN:H	1:48:A:ILE:H	1	0.19
(1,303)	1:12:A:SER:H	1:15:A:GLN:HB3	3	0.19
(1,102)	1:29:A:LEU:HA	1:33:A:ARG:HE	3	0.19
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD11	2	0.18
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD12	2	0.18
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD13	2	0.18
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD21	2	0.18
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD22	2	0.18
(1,1811)	1:41:A:LEU:HA	1:43:A:LEU:HD23	2	0.18
(1,1722)	1:29:A:LEU:HD11	1:37:A:LEU:HB2	1	0.18
(1,1722)	1:29:A:LEU:HD12	1:37:A:LEU:HB2	1	0.18
(1,1722)	1:29:A:LEU:HD13	1:37:A:LEU:HB2	1	0.18
(1,1722)	1:29:A:LEU:HD21	1:37:A:LEU:HB2	1	0.18
(1,1722)	1:29:A:LEU:HD22	1:37:A:LEU:HB2	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1722)	1:29:A:LEU:HD23	1:37:A:LEU:HB2	1	0.18
(1,1722)	1:29:A:LEU:HD11	1:37:A:LEU:HB2	3	0.18
(1,1722)	1:29:A:LEU:HD12	1:37:A:LEU:HB2	3	0.18
(1,1722)	1:29:A:LEU:HD13	1:37:A:LEU:HB2	3	0.18
(1,1722)	1:29:A:LEU:HD21	1:37:A:LEU:HB2	3	0.18
(1,1722)	1:29:A:LEU:HD22	1:37:A:LEU:HB2	3	0.18
(1,1722)	1:29:A:LEU:HD23	1:37:A:LEU:HB2	3	0.18
(1,1606)	1:18:A:ARG:HD2	1:19:A:LEU:H	2	0.18
(1,1606)	1:18:A:ARG:HD3	1:19:A:LEU:H	2	0.18
(1,1477)	1:51:A:TRP:HB3	1:52:A:PHE:HA	3	0.18
(1,1403)	1:23:A:PHE:HD1	1:27:A:ARG:H	3	0.18
(1,1403)	1:23:A:PHE:HD2	1:27:A:ARG:H	3	0.18
(1,1295)	1:44:A:ASN:HA	1:45:A:GLU:HG2	2	0.18
(1,1206)	1:34:A:ARG:HG2	1:45:A:GLU:HA	3	0.18
(1,1206)	1:34:A:ARG:HG3	1:45:A:GLU:HA	3	0.18
(1,1162)	1:50:A:ILE:HD11	1:51:A:TRP:H	2	0.18
(1,1162)	1:50:A:ILE:HD12	1:51:A:TRP:H	2	0.18
(1,1162)	1:50:A:ILE:HD13	1:51:A:TRP:H	2	0.18
(1,1126)	1:48:A:ILE:HG21	1:51:A:TRP:HB2	1	0.18
(1,1126)	1:48:A:ILE:HG22	1:51:A:TRP:HB2	1	0.18
(1,1126)	1:48:A:ILE:HG23	1:51:A:TRP:HB2	1	0.18
(1,839)	1:51:A:TRP:HB2	1:53:A:GLN:H	1	0.18
(1,814)	1:53:A:GLN:HA	1:54:A:ASN:HA	1	0.18
(1,705)	1:23:A:PHE:HZ	1:55:A:GLU:HB2	2	0.18
(1,697)	1:11:A:PHE:HZ	1:51:A:TRP:HE1	3	0.18
(1,670)	1:48:A:ILE:HA	1:51:A:TRP:HE3	2	0.18
(1,633)	1:33:A:ARG:H	1:35:A:GLN:H	2	0.18
(1,602)	1:16:A:LEU:HB3	1:51:A:TRP:HZ2	1	0.18
(1,517)	1:15:A:GLN:H	1:16:A:LEU:HA	1	0.18
(1,410)	1:19:A:LEU:HD11	1:20:A:LYS:H	2	0.18
(1,410)	1:19:A:LEU:HD12	1:20:A:LYS:H	2	0.18
(1,410)	1:19:A:LEU:HD13	1:20:A:LYS:H	2	0.18
(1,313)	1:43:A:LEU:HB2	1:45:A:GLU:H	2	0.18
(1,313)	1:43:A:LEU:HB3	1:45:A:GLU:H	2	0.18
(1,294)	1:12:A:SER:H	1:16:A:LEU:H	1	0.18
(1,202)	1:47:A:GLN:HG2	1:47:A:GLN:HE22	2	0.18
(1,181)	1:8:A:ARG:H	1:8:A:ARG:HB2	2	0.18
(1,72)	1:17:A:ALA:H	1:18:A:ARG:H	1	0.18
(1,63)	1:44:A:ASN:H	1:45:A:GLU:H	2	0.18
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD11	2	0.17
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD12	2	0.17
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD13	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD21	2	0.17
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD22	2	0.17
(1,1808)	1:41:A:LEU:H	1:41:A:LEU:HD23	2	0.17
(1,1788)	1:37:A:LEU:HD11	1:40:A:GLU:HG2	3	0.17
(1,1788)	1:37:A:LEU:HD11	1:40:A:GLU:HG3	3	0.17
(1,1788)	1:37:A:LEU:HD12	1:40:A:GLU:HG2	3	0.17
(1,1788)	1:37:A:LEU:HD12	1:40:A:GLU:HG3	3	0.17
(1,1788)	1:37:A:LEU:HD13	1:40:A:GLU:HG2	3	0.17
(1,1788)	1:37:A:LEU:HD13	1:40:A:GLU:HG3	3	0.17
(1,1788)	1:37:A:LEU:HD21	1:40:A:GLU:HG2	3	0.17
(1,1788)	1:37:A:LEU:HD21	1:40:A:GLU:HG3	3	0.17
(1,1788)	1:37:A:LEU:HD22	1:40:A:GLU:HG2	3	0.17
(1,1788)	1:37:A:LEU:HD22	1:40:A:GLU:HG3	3	0.17
(1,1788)	1:37:A:LEU:HD23	1:40:A:GLU:HG2	3	0.17
(1,1788)	1:37:A:LEU:HD23	1:40:A:GLU:HG3	3	0.17
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD11	1	0.17
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD12	1	0.17
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD13	1	0.17
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD21	1	0.17
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD22	1	0.17
(1,1764)	1:33:A:ARG:HD2	1:37:A:LEU:HD23	1	0.17
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD11	1	0.17
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD12	1	0.17
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD13	1	0.17
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD21	1	0.17
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD22	1	0.17
(1,1764)	1:33:A:ARG:HD3	1:37:A:LEU:HD23	1	0.17
(1,1648)	1:23:A:PHE:HA	1:26:A:ASN:HB2	1	0.17
(1,1648)	1:23:A:PHE:HA	1:26:A:ASN:HB3	1	0.17
(1,1606)	1:18:A:ARG:HD2	1:19:A:LEU:H	1	0.17
(1,1606)	1:18:A:ARG:HD3	1:19:A:LEU:H	1	0.17
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD11	1	0.17
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD12	1	0.17
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD13	1	0.17
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD21	1	0.17
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD22	1	0.17
(1,1579)	1:15:A:GLN:HE21	1:41:A:LEU:HD23	1	0.17
(1,1471)	1:23:A:PHE:HD1	1:56:A:ARG:H	2	0.17
(1,1471)	1:23:A:PHE:HD2	1:56:A:ARG:H	2	0.17
(1,1361)	1:57:A:ALA:H	1:59:A:ILE:H	2	0.17
(1,1237)	1:42:A:GLY:H	1:43:A:LEU:HB2	3	0.17
(1,1237)	1:42:A:GLY:H	1:43:A:LEU:HB3	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:10:A:ALA:HB1	1:11:A:PHE:HA	3	0.17
(1,1183)	1:10:A:ALA:HB2	1:11:A:PHE:HA	3	0.17
(1,1183)	1:10:A:ALA:HB3	1:11:A:PHE:HA	3	0.17
(1,1057)	1:19:A:LEU:HD21	1:48:A:ILE:H	3	0.17
(1,1057)	1:19:A:LEU:HD22	1:48:A:ILE:H	3	0.17
(1,1057)	1:19:A:LEU:HD23	1:48:A:ILE:H	3	0.17
(1,1051)	1:11:A:PHE:HA	1:43:A:LEU:HD11	2	0.17
(1,1051)	1:11:A:PHE:HA	1:43:A:LEU:HD12	2	0.17
(1,1051)	1:11:A:PHE:HA	1:43:A:LEU:HD13	2	0.17
(1,1005)	1:60:A:LYS:H	1:60:A:LYS:HD2	2	0.17
(1,1005)	1:60:A:LYS:H	1:60:A:LYS:HD3	2	0.17
(1,818)	1:48:A:ILE:HA	1:51:A:TRP:HD1	2	0.17
(1,731)	1:20:A:LYS:HA	1:23:A:PHE:HD1	3	0.17
(1,731)	1:20:A:LYS:HA	1:23:A:PHE:HD2	3	0.17
(1,720)	1:23:A:PHE:HD1	1:27:A:ARG:HB2	1	0.17
(1,720)	1:23:A:PHE:HD2	1:27:A:ARG:HB2	1	0.17
(1,670)	1:48:A:ILE:HA	1:51:A:TRP:HE3	1	0.17
(1,559)	1:29:A:LEU:H	1:52:A:PHE:HD1	3	0.17
(1,559)	1:29:A:LEU:H	1:52:A:PHE:HD2	3	0.17
(1,508)	1:19:A:LEU:HD11	1:52:A:PHE:HD1	3	0.17
(1,508)	1:19:A:LEU:HD11	1:52:A:PHE:HD2	3	0.17
(1,508)	1:19:A:LEU:HD12	1:52:A:PHE:HD1	3	0.17
(1,508)	1:19:A:LEU:HD12	1:52:A:PHE:HD2	3	0.17
(1,508)	1:19:A:LEU:HD13	1:52:A:PHE:HD1	3	0.17
(1,508)	1:19:A:LEU:HD13	1:52:A:PHE:HD2	3	0.17
(1,377)	1:37:A:LEU:H	1:40:A:GLU:H	2	0.17
(1,365)	1:50:A:ILE:HB	1:52:A:PHE:H	3	0.17
(1,325)	1:20:A:LYS:HD2	1:23:A:PHE:H	1	0.17
(1,325)	1:20:A:LYS:HD3	1:23:A:PHE:H	1	0.17
(1,317)	1:45:A:GLU:H	1:46:A:ALA:HA	3	0.17
(1,300)	1:12:A:SER:H	1:15:A:GLN:HA	1	0.17
(1,190)	1:23:A:PHE:HB2	1:51:A:TRP:HE3	3	0.17
(1,109)	1:23:A:PHE:HD1	1:26:A:ASN:H	1	0.17
(1,109)	1:23:A:PHE:HD2	1:26:A:ASN:H	1	0.17
(1,34)	1:16:A:LEU:HD11	1:51:A:TRP:HH2	3	0.17
(1,34)	1:16:A:LEU:HD12	1:51:A:TRP:HH2	3	0.17
(1,34)	1:16:A:LEU:HD13	1:51:A:TRP:HH2	3	0.17
(1,1880)	1:55:A:GLU:HA	1:58:A:LYS:HG2	1	0.16
(1,1880)	1:55:A:GLU:HA	1:58:A:LYS:HG3	1	0.16
(1,1747)	1:32:A:ARG:HA	1:32:A:ARG:HG2	1	0.16
(1,1747)	1:32:A:ARG:HA	1:32:A:ARG:HG3	1	0.16
(1,1732)	1:29:A:LEU:HD11	1:51:A:TRP:HE3	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1732)	1:29:A:LEU:HD12	1:51:A:TRP:HE3	1	0.16
(1,1732)	1:29:A:LEU:HD13	1:51:A:TRP:HE3	1	0.16
(1,1732)	1:29:A:LEU:HD21	1:51:A:TRP:HE3	1	0.16
(1,1732)	1:29:A:LEU:HD22	1:51:A:TRP:HE3	1	0.16
(1,1732)	1:29:A:LEU:HD23	1:51:A:TRP:HE3	1	0.16
(1,1700)	1:27:A:ARG:HD2	1:28:A:TYR:HE1	1	0.16
(1,1700)	1:27:A:ARG:HD2	1:28:A:TYR:HE2	1	0.16
(1,1700)	1:27:A:ARG:HD3	1:28:A:TYR:HE1	1	0.16
(1,1700)	1:27:A:ARG:HD3	1:28:A:TYR:HE2	1	0.16
(1,1506)	1:8:A:ARG:HG2	1:9:A:THR:H	1	0.16
(1,1506)	1:8:A:ARG:HG3	1:9:A:THR:H	1	0.16
(1,1442)	1:50:A:ILE:HG13	1:51:A:TRP:H	3	0.16
(1,1421)	1:52:A:PHE:HA	1:55:A:GLU:HA	2	0.16
(1,1373)	1:23:A:PHE:HE1	1:27:A:ARG:HD2	2	0.16
(1,1373)	1:23:A:PHE:HE2	1:27:A:ARG:HD2	2	0.16
(1,1363)	1:18:A:ARG:H	1:21:A:ARG:H	2	0.16
(1,1225)	1:37:A:LEU:HG	1:52:A:PHE:HE1	3	0.16
(1,1225)	1:37:A:LEU:HG	1:52:A:PHE:HE2	3	0.16
(1,1220)	1:11:A:PHE:HD1	1:43:A:LEU:HB2	1	0.16
(1,1220)	1:11:A:PHE:HD1	1:43:A:LEU:HB3	1	0.16
(1,1220)	1:11:A:PHE:HD2	1:43:A:LEU:HB2	1	0.16
(1,1220)	1:11:A:PHE:HD2	1:43:A:LEU:HB3	1	0.16
(1,1141)	1:50:A:ILE:HG21	1:54:A:ASN:HA	2	0.16
(1,1141)	1:50:A:ILE:HG22	1:54:A:ASN:HA	2	0.16
(1,1141)	1:50:A:ILE:HG23	1:54:A:ASN:HA	2	0.16
(1,1118)	1:34:A:ARG:HB3	1:48:A:ILE:HG21	2	0.16
(1,1118)	1:34:A:ARG:HB3	1:48:A:ILE:HG22	2	0.16
(1,1118)	1:34:A:ARG:HB3	1:48:A:ILE:HG23	2	0.16
(1,1043)	1:29:A:LEU:HD11	1:33:A:ARG:HE	1	0.16
(1,1043)	1:29:A:LEU:HD12	1:33:A:ARG:HE	1	0.16
(1,1043)	1:29:A:LEU:HD13	1:33:A:ARG:HE	1	0.16
(1,910)	1:37:A:LEU:H	1:37:A:LEU:HB3	3	0.16
(1,896)	1:34:A:ARG:HD2	1:45:A:GLU:HG3	3	0.16
(1,839)	1:51:A:TRP:HB2	1:53:A:GLN:H	3	0.16
(1,817)	1:11:A:PHE:HD1	1:15:A:GLN:HA	2	0.16
(1,817)	1:11:A:PHE:HD2	1:15:A:GLN:HA	2	0.16
(1,779)	1:55:A:GLU:HA	1:58:A:LYS:HB3	2	0.16
(1,779)	1:55:A:GLU:HA	1:58:A:LYS:HB3	3	0.16
(1,722)	1:23:A:PHE:HE1	1:27:A:ARG:HB2	1	0.16
(1,722)	1:23:A:PHE:HE2	1:27:A:ARG:HB2	1	0.16
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD21	3	0.16
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD22	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD23	3	0.16
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD21	3	0.16
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD22	3	0.16
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD23	3	0.16
(1,694)	1:23:A:PHE:HE1	1:28:A:TYR:H	2	0.16
(1,694)	1:23:A:PHE:HE2	1:28:A:TYR:H	2	0.16
(1,644)	1:19:A:LEU:HD11	1:51:A:TRP:HZ2	1	0.16
(1,644)	1:19:A:LEU:HD12	1:51:A:TRP:HZ2	1	0.16
(1,644)	1:19:A:LEU:HD13	1:51:A:TRP:HZ2	1	0.16
(1,567)	1:52:A:PHE:H	1:52:A:PHE:HE1	1	0.16
(1,567)	1:52:A:PHE:H	1:52:A:PHE:HE2	1	0.16
(1,567)	1:52:A:PHE:H	1:52:A:PHE:HE1	2	0.16
(1,567)	1:52:A:PHE:H	1:52:A:PHE:HE2	2	0.16
(1,535)	1:41:A:LEU:HD11	1:42:A:GLY:H	3	0.16
(1,535)	1:41:A:LEU:HD12	1:42:A:GLY:H	3	0.16
(1,535)	1:41:A:LEU:HD13	1:42:A:GLY:H	3	0.16
(1,426)	1:19:A:LEU:HD21	1:20:A:LYS:H	3	0.16
(1,426)	1:19:A:LEU:HD22	1:20:A:LYS:H	3	0.16
(1,426)	1:19:A:LEU:HD23	1:20:A:LYS:H	3	0.16
(1,398)	1:46:A:ALA:H	1:50:A:ILE:HD11	1	0.16
(1,398)	1:46:A:ALA:H	1:50:A:ILE:HD12	1	0.16
(1,398)	1:46:A:ALA:H	1:50:A:ILE:HD13	1	0.16
(1,353)	1:7:A:PRO:HD3	1:8:A:ARG:H	1	0.16
(1,314)	1:45:A:GLU:H	1:48:A:ILE:HB	3	0.16
(1,288)	1:45:A:GLU:H	1:47:A:GLN:H	1	0.16
(1,9)	1:14:A:GLU:H	1:17:A:ALA:H	1	0.16
(1,1861)	1:52:A:PHE:HA	1:55:A:GLU:HG2	1	0.15
(1,1861)	1:52:A:PHE:HA	1:55:A:GLU:HG3	1	0.15
(1,1798)	1:38:A:SER:HB2	1:43:A:LEU:HD11	3	0.15
(1,1798)	1:38:A:SER:HB2	1:43:A:LEU:HD12	3	0.15
(1,1798)	1:38:A:SER:HB2	1:43:A:LEU:HD13	3	0.15
(1,1798)	1:38:A:SER:HB2	1:43:A:LEU:HD21	3	0.15
(1,1798)	1:38:A:SER:HB2	1:43:A:LEU:HD22	3	0.15
(1,1798)	1:38:A:SER:HB2	1:43:A:LEU:HD23	3	0.15
(1,1798)	1:38:A:SER:HB3	1:43:A:LEU:HD11	3	0.15
(1,1798)	1:38:A:SER:HB3	1:43:A:LEU:HD12	3	0.15
(1,1798)	1:38:A:SER:HB3	1:43:A:LEU:HD13	3	0.15
(1,1798)	1:38:A:SER:HB3	1:43:A:LEU:HD21	3	0.15
(1,1798)	1:38:A:SER:HB3	1:43:A:LEU:HD22	3	0.15
(1,1798)	1:38:A:SER:HB3	1:43:A:LEU:HD23	3	0.15
(1,1609)	1:18:A:ARG:HD2	1:22:A:GLU:H	2	0.15
(1,1609)	1:18:A:ARG:HD3	1:22:A:GLU:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1543)	1:12:A:SER:HB2	1:15:A:GLN:HE21	2	0.15
(1,1543)	1:12:A:SER:HB3	1:15:A:GLN:HE21	2	0.15
(1,1521)	1:11:A:PHE:HD1	1:16:A:LEU:HD11	1	0.15
(1,1521)	1:11:A:PHE:HD1	1:16:A:LEU:HD12	1	0.15
(1,1521)	1:11:A:PHE:HD1	1:16:A:LEU:HD13	1	0.15
(1,1521)	1:11:A:PHE:HD1	1:16:A:LEU:HD21	1	0.15
(1,1521)	1:11:A:PHE:HD1	1:16:A:LEU:HD22	1	0.15
(1,1521)	1:11:A:PHE:HD1	1:16:A:LEU:HD23	1	0.15
(1,1521)	1:11:A:PHE:HD2	1:16:A:LEU:HD11	1	0.15
(1,1521)	1:11:A:PHE:HD2	1:16:A:LEU:HD12	1	0.15
(1,1521)	1:11:A:PHE:HD2	1:16:A:LEU:HD13	1	0.15
(1,1521)	1:11:A:PHE:HD2	1:16:A:LEU:HD21	1	0.15
(1,1521)	1:11:A:PHE:HD2	1:16:A:LEU:HD22	1	0.15
(1,1521)	1:11:A:PHE:HD2	1:16:A:LEU:HD23	1	0.15
(1,1488)	1:4:A:GLU:HB2	1:5:A:LYS:H	3	0.15
(1,1488)	1:4:A:GLU:HB3	1:5:A:LYS:H	3	0.15
(1,1480)	1:19:A:LEU:HG	1:51:A:TRP:HE3	2	0.15
(1,1144)	1:59:A:ILE:HG21	1:61:A:LYS:HA	2	0.15
(1,1144)	1:59:A:ILE:HG22	1:61:A:LYS:HA	2	0.15
(1,1144)	1:59:A:ILE:HG23	1:61:A:LYS:HA	2	0.15
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD21	3	0.15
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD22	3	0.15
(1,1080)	1:22:A:GLU:HG2	1:41:A:LEU:HD23	3	0.15
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD21	3	0.15
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD22	3	0.15
(1,1080)	1:22:A:GLU:HG3	1:41:A:LEU:HD23	3	0.15
(1,1075)	1:47:A:GLN:HB3	1:50:A:ILE:HD11	2	0.15
(1,1075)	1:47:A:GLN:HB3	1:50:A:ILE:HD12	2	0.15
(1,1075)	1:47:A:GLN:HB3	1:50:A:ILE:HD13	2	0.15
(1,1068)	1:19:A:LEU:HD21	1:51:A:TRP:HB2	1	0.15
(1,1068)	1:19:A:LEU:HD22	1:51:A:TRP:HB2	1	0.15
(1,1068)	1:19:A:LEU:HD23	1:51:A:TRP:HB2	1	0.15
(1,920)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.15
(1,880)	1:22:A:GLU:HG2	1:37:A:LEU:HA	3	0.15
(1,880)	1:22:A:GLU:HG3	1:37:A:LEU:HA	3	0.15
(1,875)	1:48:A:ILE:HG21	1:49:A:LYS:HA	2	0.15
(1,875)	1:48:A:ILE:HG22	1:49:A:LYS:HA	2	0.15
(1,875)	1:48:A:ILE:HG23	1:49:A:LYS:HA	2	0.15
(1,694)	1:23:A:PHE:HE1	1:28:A:TYR:H	3	0.15
(1,694)	1:23:A:PHE:HE2	1:28:A:TYR:H	3	0.15
(1,660)	1:22:A:GLU:HG2	1:52:A:PHE:HZ	2	0.15
(1,660)	1:22:A:GLU:HG3	1:52:A:PHE:HZ	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:11:A:PHE:HZ	1:47:A:GLN:HG3	3	0.15
(1,609)	1:11:A:PHE:HD1	1:16:A:LEU:HB2	2	0.15
(1,609)	1:11:A:PHE:HD2	1:16:A:LEU:HB2	2	0.15
(1,590)	1:45:A:GLU:HA	1:48:A:ILE:H	3	0.15
(1,559)	1:29:A:LEU:H	1:52:A:PHE:HD1	1	0.15
(1,559)	1:29:A:LEU:H	1:52:A:PHE:HD2	1	0.15
(1,527)	1:23:A:PHE:HZ	1:56:A:ARG:HE	1	0.15
(1,451)	1:17:A:ALA:H	1:20:A:LYS:H	3	0.15
(1,416)	1:22:A:GLU:H	1:23:A:PHE:HA	2	0.15
(1,415)	1:5:A:LYS:HA	1:6:A:ARG:H	1	0.15
(1,402)	1:34:A:ARG:H	1:35:A:GLN:HG3	2	0.15
(1,320)	1:45:A:GLU:H	1:48:A:ILE:H	3	0.15
(1,228)	1:43:A:LEU:H	1:44:A:ASN:H	3	0.15
(1,181)	1:8:A:ARG:H	1:8:A:ARG:HB2	3	0.15
(1,101)	1:24:A:ASN:H	1:24:A:ASN:HD21	3	0.15
(1,1859)	1:51:A:TRP:HZ2	1:55:A:GLU:HG2	2	0.14
(1,1859)	1:51:A:TRP:HZ2	1:55:A:GLU:HG3	2	0.14
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD11	3	0.14
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD12	3	0.14
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD13	3	0.14
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD21	3	0.14
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD22	3	0.14
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD23	3	0.14
(1,1708)	1:29:A:LEU:HD11	1:30:A:THR:H	1	0.14
(1,1708)	1:29:A:LEU:HD12	1:30:A:THR:H	1	0.14
(1,1708)	1:29:A:LEU:HD13	1:30:A:THR:H	1	0.14
(1,1708)	1:29:A:LEU:HD21	1:30:A:THR:H	1	0.14
(1,1708)	1:29:A:LEU:HD22	1:30:A:THR:H	1	0.14
(1,1708)	1:29:A:LEU:HD23	1:30:A:THR:H	1	0.14
(1,1687)	1:26:A:ASN:HD21	1:27:A:ARG:H	1	0.14
(1,1687)	1:26:A:ASN:HD22	1:27:A:ARG:H	1	0.14
(1,1678)	1:26:A:ASN:H	1:26:A:ASN:HD21	3	0.14
(1,1678)	1:26:A:ASN:H	1:26:A:ASN:HD22	3	0.14
(1,1606)	1:18:A:ARG:HD2	1:19:A:LEU:H	3	0.14
(1,1606)	1:18:A:ARG:HD3	1:19:A:LEU:H	3	0.14
(1,1522)	1:11:A:PHE:HD1	1:41:A:LEU:HD11	1	0.14
(1,1522)	1:11:A:PHE:HD1	1:41:A:LEU:HD12	1	0.14
(1,1522)	1:11:A:PHE:HD1	1:41:A:LEU:HD13	1	0.14
(1,1522)	1:11:A:PHE:HD1	1:41:A:LEU:HD21	1	0.14
(1,1522)	1:11:A:PHE:HD1	1:41:A:LEU:HD22	1	0.14
(1,1522)	1:11:A:PHE:HD1	1:41:A:LEU:HD23	1	0.14
(1,1522)	1:11:A:PHE:HD2	1:41:A:LEU:HD11	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1522)	1:11:A:PHE:HD2	1:41:A:LEU:HD12	1	0.14
(1,1522)	1:11:A:PHE:HD2	1:41:A:LEU:HD13	1	0.14
(1,1522)	1:11:A:PHE:HD2	1:41:A:LEU:HD21	1	0.14
(1,1522)	1:11:A:PHE:HD2	1:41:A:LEU:HD22	1	0.14
(1,1522)	1:11:A:PHE:HD2	1:41:A:LEU:HD23	1	0.14
(1,1462)	1:41:A:LEU:H	1:42:A:GLY:HA2	2	0.14
(1,1401)	1:20:A:LYS:H	1:23:A:PHE:HB3	1	0.14
(1,1401)	1:20:A:LYS:H	1:23:A:PHE:HB3	2	0.14
(1,1357)	1:16:A:LEU:HA	1:20:A:LYS:HB2	3	0.14
(1,1345)	1:20:A:LYS:HE2	1:51:A:TRP:HE1	2	0.14
(1,1345)	1:20:A:LYS:HE3	1:51:A:TRP:HE1	2	0.14
(1,1329)	1:23:A:PHE:HB2	1:51:A:TRP:HZ2	2	0.14
(1,1308)	1:19:A:LEU:HB2	1:22:A:GLU:HG2	1	0.14
(1,1308)	1:19:A:LEU:HB2	1:22:A:GLU:HG3	1	0.14
(1,1308)	1:19:A:LEU:HB3	1:22:A:GLU:HG2	1	0.14
(1,1308)	1:19:A:LEU:HB3	1:22:A:GLU:HG3	1	0.14
(1,1181)	1:28:A:TYR:HA	1:29:A:LEU:HB2	1	0.14
(1,1082)	1:19:A:LEU:HB2	1:23:A:PHE:HB3	2	0.14
(1,1082)	1:19:A:LEU:HB3	1:23:A:PHE:HB3	2	0.14
(1,1075)	1:47:A:GLN:HB3	1:50:A:ILE:HD11	3	0.14
(1,1075)	1:47:A:GLN:HB3	1:50:A:ILE:HD12	3	0.14
(1,1075)	1:47:A:GLN:HB3	1:50:A:ILE:HD13	3	0.14
(1,950)	1:35:A:GLN:HA	1:35:A:GLN:HG3	1	0.14
(1,910)	1:37:A:LEU:H	1:37:A:LEU:HB3	1	0.14
(1,821)	1:23:A:PHE:HB3	1:51:A:TRP:HZ2	1	0.14
(1,768)	1:29:A:LEU:HG	1:34:A:ARG:HA	2	0.14
(1,750)	1:11:A:PHE:HD1	1:15:A:GLN:HE22	2	0.14
(1,750)	1:11:A:PHE:HD2	1:15:A:GLN:HE22	2	0.14
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD21	2	0.14
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD22	2	0.14
(1,708)	1:11:A:PHE:HD1	1:43:A:LEU:HD23	2	0.14
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD21	2	0.14
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD22	2	0.14
(1,708)	1:11:A:PHE:HD2	1:43:A:LEU:HD23	2	0.14
(1,693)	1:24:A:ASN:H	1:52:A:PHE:HZ	3	0.14
(1,543)	1:30:A:THR:HA	1:33:A:ARG:H	3	0.14
(1,477)	1:47:A:GLN:H	1:48:A:ILE:HA	3	0.14
(1,377)	1:37:A:LEU:H	1:40:A:GLU:H	3	0.14
(1,357)	1:44:A:ASN:H	1:47:A:GLN:HG2	2	0.14
(1,267)	1:11:A:PHE:H	1:12:A:SER:H	2	0.14
(1,254)	1:4:A:GLU:H	1:4:A:GLU:HG2	1	0.14
(1,254)	1:4:A:GLU:H	1:4:A:GLU:HG3	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1873)	1:54:A:ASN:HB2	1:55:A:GLU:H	2	0.13
(1,1873)	1:54:A:ASN:HB3	1:55:A:GLU:H	2	0.13
(1,1802)	1:38:A:SER:HB2	1:48:A:ILE:HG12	1	0.13
(1,1802)	1:38:A:SER:HB2	1:48:A:ILE:HG13	1	0.13
(1,1802)	1:38:A:SER:HB3	1:48:A:ILE:HG12	1	0.13
(1,1802)	1:38:A:SER:HB3	1:48:A:ILE:HG13	1	0.13
(1,1668)	1:24:A:ASN:HD21	1:25:A:GLU:H	3	0.13
(1,1668)	1:24:A:ASN:HD22	1:25:A:GLU:H	3	0.13
(1,1493)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	0.13
(1,1493)	1:6:A:ARG:H	1:6:A:ARG:HB3	1	0.13
(1,1443)	1:56:A:ARG:H	1:56:A:ARG:HG2	2	0.13
(1,1397)	1:19:A:LEU:HD11	1:48:A:ILE:H	3	0.13
(1,1397)	1:19:A:LEU:HD12	1:48:A:ILE:H	3	0.13
(1,1397)	1:19:A:LEU:HD13	1:48:A:ILE:H	3	0.13
(1,1389)	1:35:A:GLN:HE21	1:36:A:GLN:HG2	1	0.13
(1,1389)	1:35:A:GLN:HE21	1:36:A:GLN:HG3	1	0.13
(1,1357)	1:16:A:LEU:HA	1:20:A:LYS:HB2	2	0.13
(1,1273)	1:14:A:GLU:HB2	1:15:A:GLN:H	1	0.13
(1,1212)	1:29:A:LEU:HA	1:30:A:THR:HG21	2	0.13
(1,1212)	1:29:A:LEU:HA	1:30:A:THR:HG22	2	0.13
(1,1212)	1:29:A:LEU:HA	1:30:A:THR:HG23	2	0.13
(1,1142)	1:9:A:THR:HG21	1:10:A:ALA:HA	3	0.13
(1,1142)	1:9:A:THR:HG22	1:10:A:ALA:HA	3	0.13
(1,1142)	1:9:A:THR:HG23	1:10:A:ALA:HA	3	0.13
(1,1082)	1:19:A:LEU:HB2	1:23:A:PHE:HB3	1	0.13
(1,1082)	1:19:A:LEU:HB3	1:23:A:PHE:HB3	1	0.13
(1,1043)	1:29:A:LEU:HD11	1:33:A:ARG:HE	2	0.13
(1,1043)	1:29:A:LEU:HD12	1:33:A:ARG:HE	2	0.13
(1,1043)	1:29:A:LEU:HD13	1:33:A:ARG:HE	2	0.13
(1,950)	1:35:A:GLN:HA	1:35:A:GLN:HG3	2	0.13
(1,854)	1:37:A:LEU:H	1:38:A:SER:HA	3	0.13
(1,838)	1:51:A:TRP:H	1:52:A:PHE:HA	1	0.13
(1,829)	1:51:A:TRP:HB2	1:51:A:TRP:HE3	1	0.13
(1,799)	1:45:A:GLU:HA	1:46:A:ALA:HA	1	0.13
(1,790)	1:51:A:TRP:HA	1:55:A:GLU:HA	2	0.13
(1,784)	1:15:A:GLN:HA	1:41:A:LEU:HB2	2	0.13
(1,715)	1:23:A:PHE:HZ	1:59:A:ILE:HD11	2	0.13
(1,715)	1:23:A:PHE:HZ	1:59:A:ILE:HD12	2	0.13
(1,715)	1:23:A:PHE:HZ	1:59:A:ILE:HD13	2	0.13
(1,713)	1:11:A:PHE:HD1	1:16:A:LEU:HD11	2	0.13
(1,713)	1:11:A:PHE:HD1	1:16:A:LEU:HD12	2	0.13
(1,713)	1:11:A:PHE:HD1	1:16:A:LEU:HD13	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,713)	1:11:A:PHE:HD2	1:16:A:LEU:HD11	2	0.13
(1,713)	1:11:A:PHE:HD2	1:16:A:LEU:HD12	2	0.13
(1,713)	1:11:A:PHE:HD2	1:16:A:LEU:HD13	2	0.13
(1,709)	1:43:A:LEU:HD21	1:47:A:GLN:HE22	1	0.13
(1,709)	1:43:A:LEU:HD22	1:47:A:GLN:HE22	1	0.13
(1,709)	1:43:A:LEU:HD23	1:47:A:GLN:HE22	1	0.13
(1,709)	1:43:A:LEU:HD21	1:47:A:GLN:HE22	2	0.13
(1,709)	1:43:A:LEU:HD22	1:47:A:GLN:HE22	2	0.13
(1,709)	1:43:A:LEU:HD23	1:47:A:GLN:HE22	2	0.13
(1,707)	1:29:A:LEU:HD21	1:51:A:TRP:HE3	3	0.13
(1,707)	1:29:A:LEU:HD22	1:51:A:TRP:HE3	3	0.13
(1,707)	1:29:A:LEU:HD23	1:51:A:TRP:HE3	3	0.13
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD11	2	0.13
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD12	2	0.13
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD13	2	0.13
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD11	3	0.13
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD12	3	0.13
(1,640)	1:11:A:PHE:HZ	1:19:A:LEU:HD13	3	0.13
(1,639)	1:19:A:LEU:HD11	1:52:A:PHE:HE1	2	0.13
(1,639)	1:19:A:LEU:HD11	1:52:A:PHE:HE2	2	0.13
(1,639)	1:19:A:LEU:HD12	1:52:A:PHE:HE1	2	0.13
(1,639)	1:19:A:LEU:HD12	1:52:A:PHE:HE2	2	0.13
(1,639)	1:19:A:LEU:HD13	1:52:A:PHE:HE1	2	0.13
(1,639)	1:19:A:LEU:HD13	1:52:A:PHE:HE2	2	0.13
(1,631)	1:23:A:PHE:HD1	1:55:A:GLU:H	1	0.13
(1,631)	1:23:A:PHE:HD2	1:55:A:GLU:H	1	0.13
(1,512)	1:23:A:PHE:HB2	1:24:A:ASN:H	2	0.13
(1,443)	1:38:A:SER:H	1:40:A:GLU:H	1	0.13
(1,398)	1:46:A:ALA:H	1:50:A:ILE:HD11	3	0.13
(1,398)	1:46:A:ALA:H	1:50:A:ILE:HD12	3	0.13
(1,398)	1:46:A:ALA:H	1:50:A:ILE:HD13	3	0.13
(1,309)	1:12:A:SER:H	1:16:A:LEU:HD11	3	0.13
(1,309)	1:12:A:SER:H	1:16:A:LEU:HD12	3	0.13
(1,309)	1:12:A:SER:H	1:16:A:LEU:HD13	3	0.13
(1,309)	1:12:A:SER:H	1:16:A:LEU:HD21	3	0.13
(1,309)	1:12:A:SER:H	1:16:A:LEU:HD22	3	0.13
(1,309)	1:12:A:SER:H	1:16:A:LEU:HD23	3	0.13
(1,210)	1:48:A:ILE:HA	1:48:A:ILE:HD11	3	0.13
(1,210)	1:48:A:ILE:HA	1:48:A:ILE:HD12	3	0.13
(1,210)	1:48:A:ILE:HA	1:48:A:ILE:HD13	3	0.13
(1,184)	1:8:A:ARG:HA	1:8:A:ARG:HD2	2	0.13
(1,184)	1:8:A:ARG:HA	1:8:A:ARG:HD3	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:15:A:GLN:HA	1:17:A:ALA:H	2	0.13
(1,4)	1:55:A:GLU:H	1:57:A:ALA:H	2	0.13
(1,1902)	1:59:A:ILE:HG21	1:61:A:LYS:HG2	2	0.12
(1,1902)	1:59:A:ILE:HG21	1:61:A:LYS:HG3	2	0.12
(1,1902)	1:59:A:ILE:HG22	1:61:A:LYS:HG2	2	0.12
(1,1902)	1:59:A:ILE:HG22	1:61:A:LYS:HG3	2	0.12
(1,1902)	1:59:A:ILE:HG23	1:61:A:LYS:HG2	2	0.12
(1,1902)	1:59:A:ILE:HG23	1:61:A:LYS:HG3	2	0.12
(1,1847)	1:50:A:ILE:H	1:53:A:GLN:HE21	3	0.12
(1,1847)	1:50:A:ILE:H	1:53:A:GLN:HE22	3	0.12
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD11	2	0.12
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD12	2	0.12
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD13	2	0.12
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD21	2	0.12
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD22	2	0.12
(1,1821)	1:43:A:LEU:H	1:43:A:LEU:HD23	2	0.12
(1,1806)	1:40:A:GLU:HB2	1:41:A:LEU:HD11	2	0.12
(1,1806)	1:40:A:GLU:HB2	1:41:A:LEU:HD12	2	0.12
(1,1806)	1:40:A:GLU:HB2	1:41:A:LEU:HD13	2	0.12
(1,1806)	1:40:A:GLU:HB2	1:41:A:LEU:HD21	2	0.12
(1,1806)	1:40:A:GLU:HB2	1:41:A:LEU:HD22	2	0.12
(1,1806)	1:40:A:GLU:HB2	1:41:A:LEU:HD23	2	0.12
(1,1806)	1:40:A:GLU:HB3	1:41:A:LEU:HD11	2	0.12
(1,1806)	1:40:A:GLU:HB3	1:41:A:LEU:HD12	2	0.12
(1,1806)	1:40:A:GLU:HB3	1:41:A:LEU:HD13	2	0.12
(1,1806)	1:40:A:GLU:HB3	1:41:A:LEU:HD21	2	0.12
(1,1806)	1:40:A:GLU:HB3	1:41:A:LEU:HD22	2	0.12
(1,1806)	1:40:A:GLU:HB3	1:41:A:LEU:HD23	2	0.12
(1,1781)	1:37:A:LEU:HA	1:41:A:LEU:HD11	1	0.12
(1,1781)	1:37:A:LEU:HA	1:41:A:LEU:HD12	1	0.12
(1,1781)	1:37:A:LEU:HA	1:41:A:LEU:HD13	1	0.12
(1,1781)	1:37:A:LEU:HA	1:41:A:LEU:HD21	1	0.12
(1,1781)	1:37:A:LEU:HA	1:41:A:LEU:HD22	1	0.12
(1,1781)	1:37:A:LEU:HA	1:41:A:LEU:HD23	1	0.12
(1,1733)	1:29:A:LEU:HD11	1:52:A:PHE:H	2	0.12
(1,1733)	1:29:A:LEU:HD12	1:52:A:PHE:H	2	0.12
(1,1733)	1:29:A:LEU:HD13	1:52:A:PHE:H	2	0.12
(1,1733)	1:29:A:LEU:HD21	1:52:A:PHE:H	2	0.12
(1,1733)	1:29:A:LEU:HD22	1:52:A:PHE:H	2	0.12
(1,1733)	1:29:A:LEU:HD23	1:52:A:PHE:H	2	0.12
(1,1708)	1:29:A:LEU:HD11	1:30:A:THR:H	3	0.12
(1,1708)	1:29:A:LEU:HD12	1:30:A:THR:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1708)	1:29:A:LEU:HD13	1:30:A:THR:H	3	0.12
(1,1708)	1:29:A:LEU:HD21	1:30:A:THR:H	3	0.12
(1,1708)	1:29:A:LEU:HD22	1:30:A:THR:H	3	0.12
(1,1708)	1:29:A:LEU:HD23	1:30:A:THR:H	3	0.12
(1,1505)	1:8:A:ARG:HB2	1:9:A:THR:HG21	2	0.12
(1,1505)	1:8:A:ARG:HB2	1:9:A:THR:HG22	2	0.12
(1,1505)	1:8:A:ARG:HB2	1:9:A:THR:HG23	2	0.12
(1,1505)	1:8:A:ARG:HB3	1:9:A:THR:HG21	2	0.12
(1,1505)	1:8:A:ARG:HB3	1:9:A:THR:HG22	2	0.12
(1,1505)	1:8:A:ARG:HB3	1:9:A:THR:HG23	2	0.12
(1,1462)	1:41:A:LEU:H	1:42:A:GLY:HA2	3	0.12
(1,1372)	1:32:A:ARG:H	1:34:A:ARG:H	1	0.12
(1,1234)	1:14:A:GLU:H	1:17:A:ALA:HB1	1	0.12
(1,1234)	1:14:A:GLU:H	1:17:A:ALA:HB2	1	0.12
(1,1234)	1:14:A:GLU:H	1:17:A:ALA:HB3	1	0.12
(1,1220)	1:11:A:PHE:HD1	1:43:A:LEU:HB2	2	0.12
(1,1220)	1:11:A:PHE:HD1	1:43:A:LEU:HB3	2	0.12
(1,1220)	1:11:A:PHE:HD2	1:43:A:LEU:HB2	2	0.12
(1,1220)	1:11:A:PHE:HD2	1:43:A:LEU:HB3	2	0.12
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD21	2	0.12
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD22	2	0.12
(1,1197)	1:19:A:LEU:HG	1:41:A:LEU:HD23	2	0.12
(1,1135)	1:37:A:LEU:HA	1:48:A:ILE:HG12	2	0.12
(1,1135)	1:37:A:LEU:HA	1:48:A:ILE:HG13	2	0.12
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD21	2	0.12
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD22	2	0.12
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD23	2	0.12
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD21	2	0.12
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD22	2	0.12
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD23	2	0.12
(1,1045)	1:29:A:LEU:HD21	1:34:A:ARG:HG2	1	0.12
(1,1045)	1:29:A:LEU:HD21	1:34:A:ARG:HG3	1	0.12
(1,1045)	1:29:A:LEU:HD22	1:34:A:ARG:HG2	1	0.12
(1,1045)	1:29:A:LEU:HD22	1:34:A:ARG:HG3	1	0.12
(1,1045)	1:29:A:LEU:HD23	1:34:A:ARG:HG2	1	0.12
(1,1045)	1:29:A:LEU:HD23	1:34:A:ARG:HG3	1	0.12
(1,939)	1:30:A:THR:H	1:30:A:THR:HG21	2	0.12
(1,939)	1:30:A:THR:H	1:30:A:THR:HG22	2	0.12
(1,939)	1:30:A:THR:H	1:30:A:THR:HG23	2	0.12
(1,925)	1:24:A:ASN:H	1:24:A:ASN:HB2	3	0.12
(1,867)	1:38:A:SER:HB3	1:45:A:GLU:HA	3	0.12
(1,859)	1:31:A:GLU:HA	1:33:A:ARG:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:33:A:ARG:H	1:35:A:GLN:H	3	0.12
(1,631)	1:23:A:PHE:HD1	1:55:A:GLU:H	2	0.12
(1,631)	1:23:A:PHE:HD2	1:55:A:GLU:H	2	0.12
(1,607)	1:43:A:LEU:HB2	1:47:A:GLN:HE22	1	0.12
(1,607)	1:43:A:LEU:HB3	1:47:A:GLN:HE22	1	0.12
(1,575)	1:29:A:LEU:HG	1:30:A:THR:H	1	0.12
(1,484)	1:47:A:GLN:H	1:48:A:ILE:HB	1	0.12
(1,441)	1:16:A:LEU:H	1:18:A:ARG:H	3	0.12
(1,365)	1:50:A:ILE:HB	1:52:A:PHE:H	1	0.12
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD11	3	0.12
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD12	3	0.12
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD13	3	0.12
(1,204)	1:41:A:LEU:HB2	1:43:A:LEU:H	3	0.12
(1,164)	1:51:A:TRP:HB3	1:51:A:TRP:HZ3	1	0.12
(1,1902)	1:59:A:ILE:HG21	1:61:A:LYS:HG2	3	0.11
(1,1902)	1:59:A:ILE:HG21	1:61:A:LYS:HG3	3	0.11
(1,1902)	1:59:A:ILE:HG22	1:61:A:LYS:HG2	3	0.11
(1,1902)	1:59:A:ILE:HG22	1:61:A:LYS:HG3	3	0.11
(1,1902)	1:59:A:ILE:HG23	1:61:A:LYS:HG2	3	0.11
(1,1902)	1:59:A:ILE:HG23	1:61:A:LYS:HG3	3	0.11
(1,1773)	1:36:A:GLN:HA	1:37:A:LEU:HD11	2	0.11
(1,1773)	1:36:A:GLN:HA	1:37:A:LEU:HD12	2	0.11
(1,1773)	1:36:A:GLN:HA	1:37:A:LEU:HD13	2	0.11
(1,1773)	1:36:A:GLN:HA	1:37:A:LEU:HD21	2	0.11
(1,1773)	1:36:A:GLN:HA	1:37:A:LEU:HD22	2	0.11
(1,1773)	1:36:A:GLN:HA	1:37:A:LEU:HD23	2	0.11
(1,1767)	1:34:A:ARG:H	1:37:A:LEU:HD11	1	0.11
(1,1767)	1:34:A:ARG:H	1:37:A:LEU:HD12	1	0.11
(1,1767)	1:34:A:ARG:H	1:37:A:LEU:HD13	1	0.11
(1,1767)	1:34:A:ARG:H	1:37:A:LEU:HD21	1	0.11
(1,1767)	1:34:A:ARG:H	1:37:A:LEU:HD22	1	0.11
(1,1767)	1:34:A:ARG:H	1:37:A:LEU:HD23	1	0.11
(1,1759)	1:33:A:ARG:HG2	1:37:A:LEU:HD11	3	0.11
(1,1759)	1:33:A:ARG:HG2	1:37:A:LEU:HD12	3	0.11
(1,1759)	1:33:A:ARG:HG2	1:37:A:LEU:HD13	3	0.11
(1,1759)	1:33:A:ARG:HG2	1:37:A:LEU:HD21	3	0.11
(1,1759)	1:33:A:ARG:HG2	1:37:A:LEU:HD22	3	0.11
(1,1759)	1:33:A:ARG:HG2	1:37:A:LEU:HD23	3	0.11
(1,1759)	1:33:A:ARG:HG3	1:37:A:LEU:HD11	3	0.11
(1,1759)	1:33:A:ARG:HG3	1:37:A:LEU:HD12	3	0.11
(1,1759)	1:33:A:ARG:HG3	1:37:A:LEU:HD13	3	0.11
(1,1759)	1:33:A:ARG:HG3	1:37:A:LEU:HD21	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1759)	1:33:A:ARG:HG3	1:37:A:LEU:HD22	3	0.11
(1,1759)	1:33:A:ARG:HG3	1:37:A:LEU:HD23	3	0.11
(1,1557)	1:14:A:GLU:HA	1:14:A:GLU:HG2	1	0.11
(1,1557)	1:14:A:GLU:HA	1:14:A:GLU:HG3	1	0.11
(1,1523)	1:11:A:PHE:HD1	1:43:A:LEU:HD11	2	0.11
(1,1523)	1:11:A:PHE:HD1	1:43:A:LEU:HD12	2	0.11
(1,1523)	1:11:A:PHE:HD1	1:43:A:LEU:HD13	2	0.11
(1,1523)	1:11:A:PHE:HD1	1:43:A:LEU:HD21	2	0.11
(1,1523)	1:11:A:PHE:HD1	1:43:A:LEU:HD22	2	0.11
(1,1523)	1:11:A:PHE:HD1	1:43:A:LEU:HD23	2	0.11
(1,1523)	1:11:A:PHE:HD2	1:43:A:LEU:HD11	2	0.11
(1,1523)	1:11:A:PHE:HD2	1:43:A:LEU:HD12	2	0.11
(1,1523)	1:11:A:PHE:HD2	1:43:A:LEU:HD13	2	0.11
(1,1523)	1:11:A:PHE:HD2	1:43:A:LEU:HD21	2	0.11
(1,1523)	1:11:A:PHE:HD2	1:43:A:LEU:HD22	2	0.11
(1,1523)	1:11:A:PHE:HD2	1:43:A:LEU:HD23	2	0.11
(1,1506)	1:8:A:ARG:HG2	1:9:A:THR:H	2	0.11
(1,1506)	1:8:A:ARG:HG3	1:9:A:THR:H	2	0.11
(1,1435)	1:49:A:LYS:HA	1:53:A:GLN:H	3	0.11
(1,1422)	1:34:A:ARG:HD2	1:46:A:ALA:HA	1	0.11
(1,1361)	1:57:A:ALA:H	1:59:A:ILE:H	3	0.11
(1,1289)	1:33:A:ARG:HA	1:36:A:GLN:HB2	3	0.11
(1,1234)	1:14:A:GLU:H	1:17:A:ALA:HB1	3	0.11
(1,1234)	1:14:A:GLU:H	1:17:A:ALA:HB2	3	0.11
(1,1234)	1:14:A:GLU:H	1:17:A:ALA:HB3	3	0.11
(1,1224)	1:10:A:ALA:HB1	1:47:A:GLN:HE21	1	0.11
(1,1224)	1:10:A:ALA:HB2	1:47:A:GLN:HE21	1	0.11
(1,1224)	1:10:A:ALA:HB3	1:47:A:GLN:HE21	1	0.11
(1,1169)	1:9:A:THR:HG21	1:16:A:LEU:HD11	2	0.11
(1,1169)	1:9:A:THR:HG21	1:16:A:LEU:HD12	2	0.11
(1,1169)	1:9:A:THR:HG21	1:16:A:LEU:HD13	2	0.11
(1,1169)	1:9:A:THR:HG22	1:16:A:LEU:HD11	2	0.11
(1,1169)	1:9:A:THR:HG22	1:16:A:LEU:HD12	2	0.11
(1,1169)	1:9:A:THR:HG22	1:16:A:LEU:HD13	2	0.11
(1,1169)	1:9:A:THR:HG23	1:16:A:LEU:HD11	2	0.11
(1,1169)	1:9:A:THR:HG23	1:16:A:LEU:HD12	2	0.11
(1,1169)	1:9:A:THR:HG23	1:16:A:LEU:HD13	2	0.11
(1,1099)	1:11:A:PHE:HD1	1:19:A:LEU:HB2	1	0.11
(1,1099)	1:11:A:PHE:HD1	1:19:A:LEU:HB3	1	0.11
(1,1099)	1:11:A:PHE:HD2	1:19:A:LEU:HB2	1	0.11
(1,1099)	1:11:A:PHE:HD2	1:19:A:LEU:HB3	1	0.11
(1,1065)	1:19:A:LEU:HD21	1:48:A:ILE:HB	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1065)	1:19:A:LEU:HD22	1:48:A:ILE:HB	3	0.11
(1,1065)	1:19:A:LEU:HD23	1:48:A:ILE:HB	3	0.11
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD21	1	0.11
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD22	1	0.11
(1,1055)	1:11:A:PHE:HD1	1:19:A:LEU:HD23	1	0.11
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD21	1	0.11
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD22	1	0.11
(1,1055)	1:11:A:PHE:HD2	1:19:A:LEU:HD23	1	0.11
(1,1014)	1:16:A:LEU:H	1:16:A:LEU:HD11	3	0.11
(1,1014)	1:16:A:LEU:H	1:16:A:LEU:HD12	3	0.11
(1,1014)	1:16:A:LEU:H	1:16:A:LEU:HD13	3	0.11
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD11	3	0.11
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD12	3	0.11
(1,993)	1:41:A:LEU:H	1:41:A:LEU:HD13	3	0.11
(1,901)	1:6:A:ARG:HD2	1:7:A:PRO:HD3	2	0.11
(1,901)	1:6:A:ARG:HD3	1:7:A:PRO:HD3	2	0.11
(1,856)	1:14:A:GLU:H	1:15:A:GLN:HA	1	0.11
(1,854)	1:37:A:LEU:H	1:38:A:SER:HA	2	0.11
(1,849)	1:16:A:LEU:H	1:17:A:ALA:HA	2	0.11
(1,829)	1:51:A:TRP:HB2	1:51:A:TRP:HE3	2	0.11
(1,630)	1:51:A:TRP:HH2	1:52:A:PHE:HE1	1	0.11
(1,630)	1:51:A:TRP:HH2	1:52:A:PHE:HE2	1	0.11
(1,625)	1:19:A:LEU:HA	1:52:A:PHE:HE1	1	0.11
(1,625)	1:19:A:LEU:HA	1:52:A:PHE:HE2	1	0.11
(1,609)	1:11:A:PHE:HD1	1:16:A:LEU:HB2	3	0.11
(1,609)	1:11:A:PHE:HD2	1:16:A:LEU:HB2	3	0.11
(1,592)	1:59:A:ILE:H	1:60:A:LYS:HA	1	0.11
(1,553)	1:51:A:TRP:HB2	1:52:A:PHE:HD1	1	0.11
(1,553)	1:51:A:TRP:HB2	1:52:A:PHE:HD2	1	0.11
(1,523)	1:29:A:LEU:HA	1:52:A:PHE:HD1	1	0.11
(1,523)	1:29:A:LEU:HA	1:52:A:PHE:HD2	1	0.11
(1,474)	1:38:A:SER:HA	1:42:A:GLY:H	3	0.11
(1,365)	1:50:A:ILE:HB	1:52:A:PHE:H	2	0.11
(1,331)	1:23:A:PHE:H	1:24:A:ASN:HA	2	0.11
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD11	1	0.11
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD12	1	0.11
(1,260)	1:16:A:LEU:HA	1:16:A:LEU:HD13	1	0.11
(1,164)	1:51:A:TRP:HB3	1:51:A:TRP:HZ3	2	0.11
(1,1878)	1:55:A:GLU:H	1:55:A:GLU:HG2	2	0.1
(1,1878)	1:55:A:GLU:H	1:55:A:GLU:HG3	2	0.1
(1,1730)	1:29:A:LEU:HD11	1:49:A:LYS:HA	3	0.1
(1,1730)	1:29:A:LEU:HD12	1:49:A:LYS:HA	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1730)	1:29:A:LEU:HD13	1:49:A:LYS:HA	3	0.1
(1,1730)	1:29:A:LEU:HD21	1:49:A:LYS:HA	3	0.1
(1,1730)	1:29:A:LEU:HD22	1:49:A:LYS:HA	3	0.1
(1,1730)	1:29:A:LEU:HD23	1:49:A:LYS:HA	3	0.1
(1,1667)	1:24:A:ASN:HB2	1:25:A:GLU:HB2	1	0.1
(1,1667)	1:24:A:ASN:HB2	1:25:A:GLU:HB3	1	0.1
(1,1667)	1:24:A:ASN:HB3	1:25:A:GLU:HB2	1	0.1
(1,1667)	1:24:A:ASN:HB3	1:25:A:GLU:HB3	1	0.1
(1,1440)	1:8:A:ARG:HG3	1:9:A:THR:H	2	0.1
(1,1398)	1:17:A:ALA:H	1:19:A:LEU:HD11	3	0.1
(1,1398)	1:17:A:ALA:H	1:19:A:LEU:HD12	3	0.1
(1,1398)	1:17:A:ALA:H	1:19:A:LEU:HD13	3	0.1
(1,1355)	1:33:A:ARG:H	1:35:A:GLN:HB3	3	0.1
(1,1151)	1:15:A:GLN:HE21	1:41:A:LEU:HD21	1	0.1
(1,1151)	1:15:A:GLN:HE21	1:41:A:LEU:HD22	1	0.1
(1,1151)	1:15:A:GLN:HE21	1:41:A:LEU:HD23	1	0.1
(1,962)	1:45:A:GLU:HA	1:45:A:GLU:HG2	2	0.1
(1,900)	1:30:A:THR:H	1:33:A:ARG:HD3	2	0.1
(1,891)	1:18:A:ARG:HB2	1:37:A:LEU:HA	3	0.1
(1,891)	1:18:A:ARG:HB3	1:37:A:LEU:HA	3	0.1
(1,553)	1:51:A:TRP:HB2	1:52:A:PHE:HD1	3	0.1
(1,553)	1:51:A:TRP:HB2	1:52:A:PHE:HD2	3	0.1
(1,517)	1:15:A:GLN:H	1:16:A:LEU:HA	3	0.1
(1,499)	1:54:A:ASN:HB3	1:55:A:GLU:H	2	0.1
(1,433)	1:26:A:ASN:HB2	1:27:A:ARG:H	3	0.1
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG21	3	0.1
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG22	3	0.1
(1,397)	1:34:A:ARG:H	1:48:A:ILE:HG23	3	0.1
(1,347)	1:31:A:GLU:H	1:32:A:ARG:HA	3	0.1
(1,291)	1:34:A:ARG:HB3	1:45:A:GLU:H	1	0.1
(1,202)	1:47:A:GLN:HG2	1:47:A:GLN:HE22	1	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found