



Full wwPDB NMR Structure Validation Report ⓘ

Mar 28, 2026 – 07:14 AM UTC

PDB ID : 5TM0 / pdb_00005tm0
BMRB ID : 26821
Title : Solution NMR structures of two alternative conformations of E. coli tryptophan repressor in dynamic equilibrium
Authors : Harish, B.; Swapna, G.V.T.; Kornhaber, G.J.; Montelione, G.T.; Carey, J.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2016-10-12

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

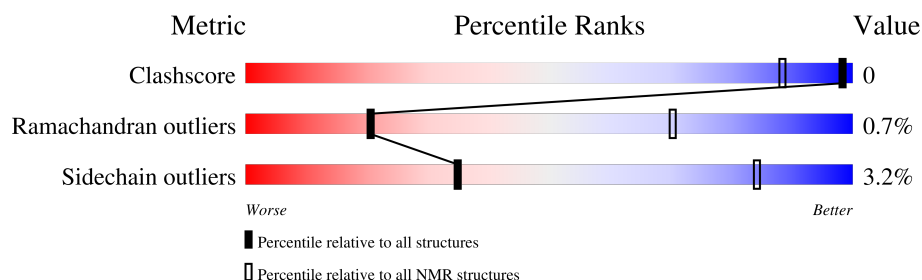
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 11%.

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	108	69% 19% 11%
1	B	108	69% 22% 8%
1	C	108	79% 19% ..
1	D	108	66% 26% . . .

2 Ensemble composition and analysis

This entry contains 15 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:11-A:106, B:10-B:108, C:1-C:106, D:5-D:108 (405)	0.84	4

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5
2	6, 7, 8, 9, 10
3	13, 14
4	11, 12
Single-model clusters	15

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6988 atoms, of which 3520 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trp operon repressor.

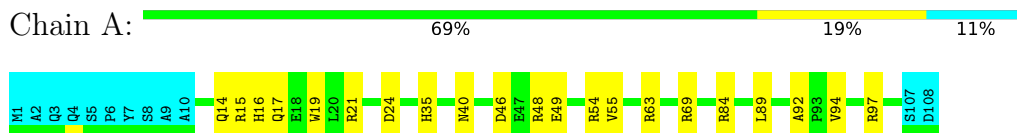
Mol	Chain	Residues	Atoms						Trace
1	A	108	Total	C	H	N	O	S	0
			1747	541	880	157	165	4	
1	B	108	Total	C	H	N	O	S	0
			1747	541	880	157	165	4	
1	C	108	Total	C	H	N	O	S	0
			1747	541	880	157	165	4	
1	D	108	Total	C	H	N	O	S	0
			1747	541	880	157	165	4	

4 Residue-property plots [i](#)

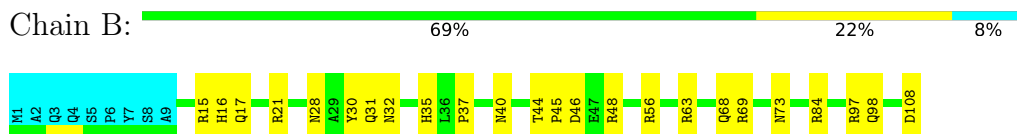
4.1 Average score per residue in the NMR ensemble

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

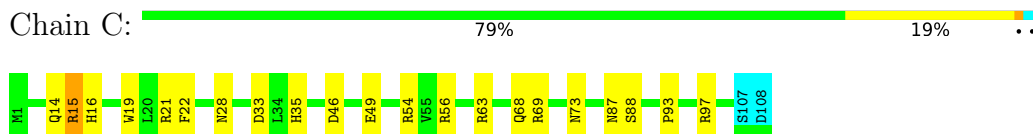
- Molecule 1: Trp operon repressor



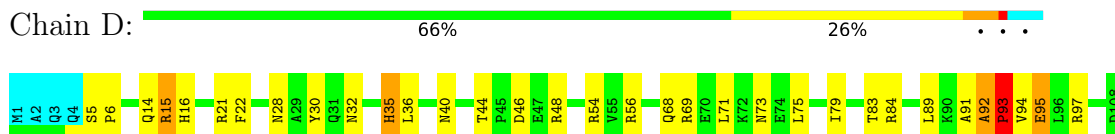
- Molecule 1: Trp operon repressor



- Molecule 1: Trp operon repressor



- Molecule 1: Trp operon repressor

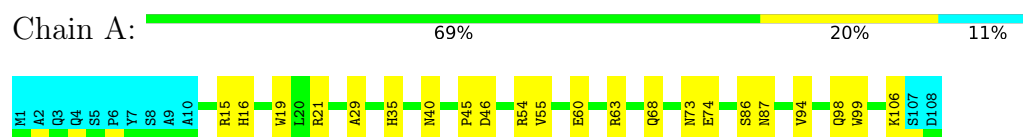


4.2 Scores per residue for each member of the ensemble

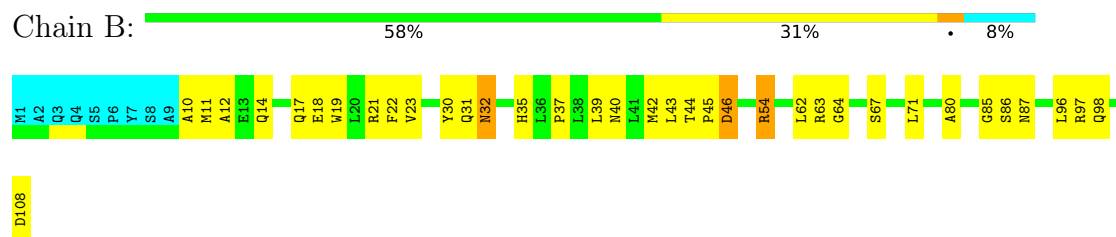
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

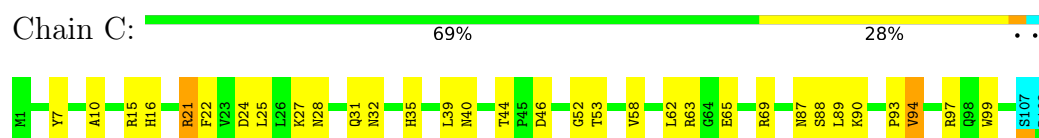
- Molecule 1: Trp operon repressor



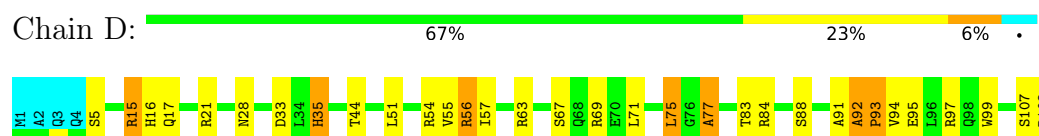
- Molecule 1: Trp operon repressor



- Molecule 1: Trp operon repressor

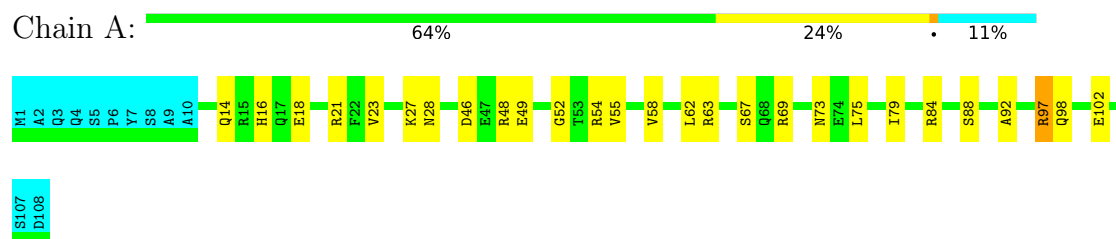


- Molecule 1: Trp operon repressor



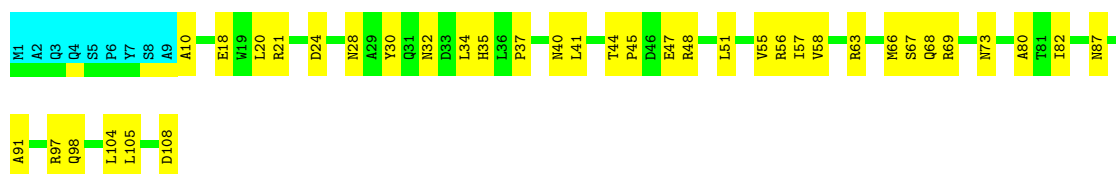
4.2.2 Score per residue for model 2

- Molecule 1: Trp operon repressor



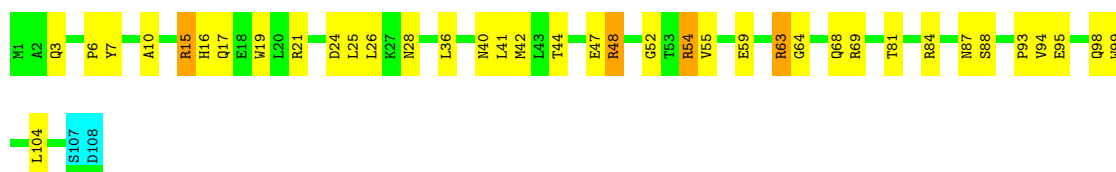
- Molecule 1: Trp operon repressor





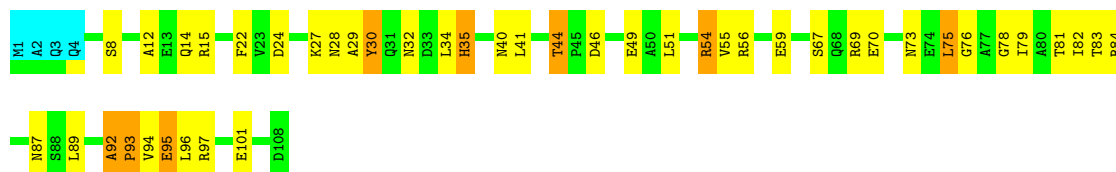
- Molecule 1: Trp operon repressor

Chain C: 63% 31%



- Molecule 1: Trp operon repressor

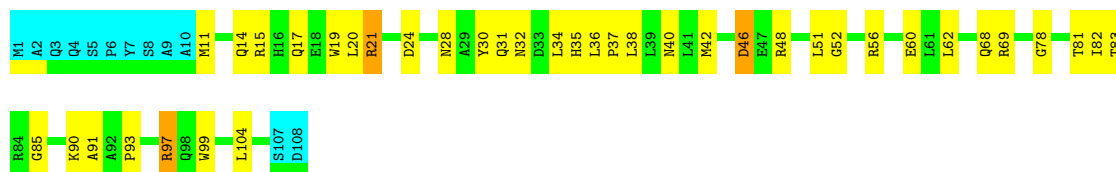
Chain D: 56% 33% 7%



4.2.3 Score per residue for model 3

- Molecule 1: Trp operon repressor

Chain A: 53% 33% 11%

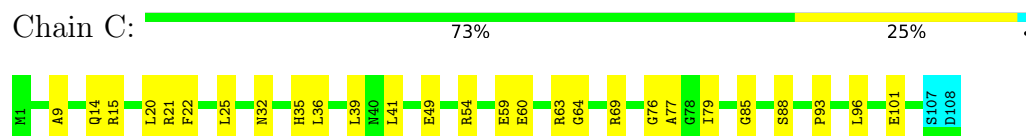


- Molecule 1: Trp operon repressor

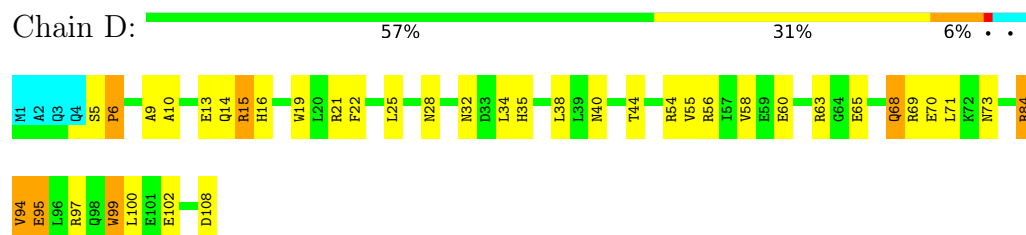
Chain B: 61% 31% 8%



- Molecule 1: Trp operon repressor

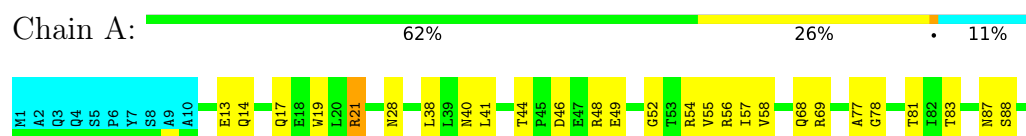


- Molecule 1: Trp operon repressor

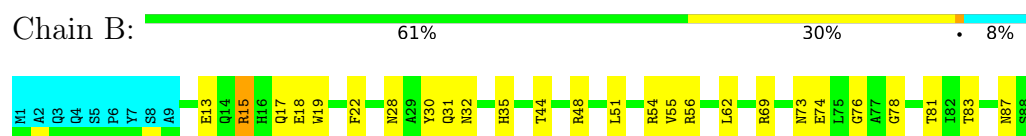


4.2.4 Score per residue for model 4 (medoid)

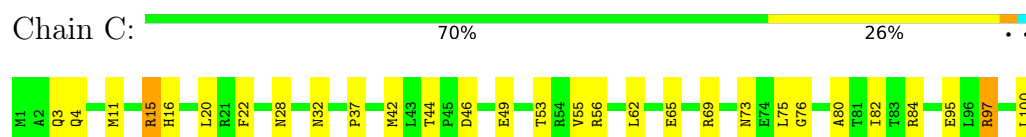
- Molecule 1: Trp operon repressor



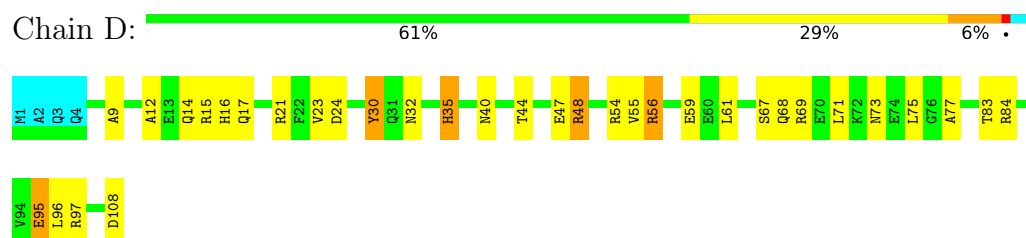
- Molecule 1: Trp operon repressor



- Molecule 1: Trp operon repressor

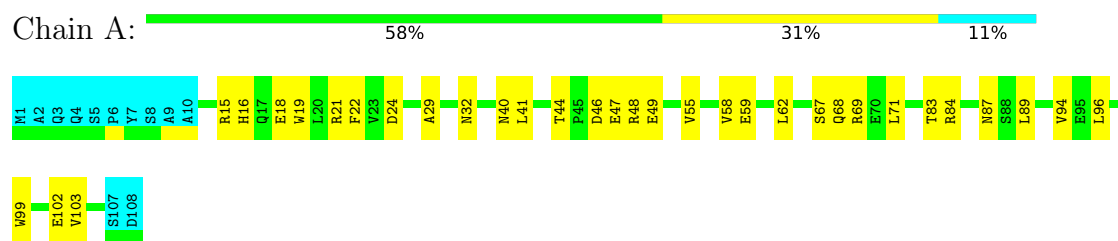


- Molecule 1: Trp operon repressor

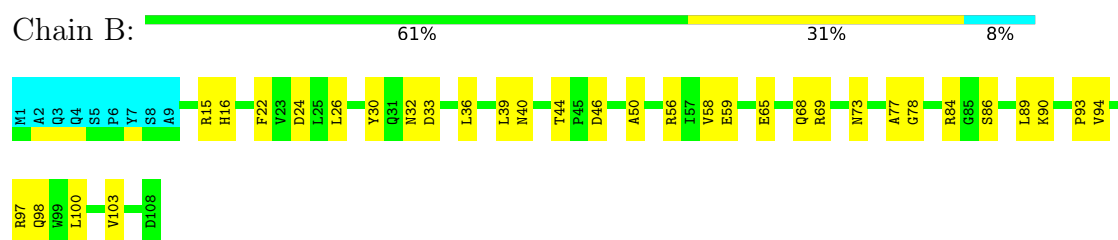


4.2.5 Score per residue for model 5

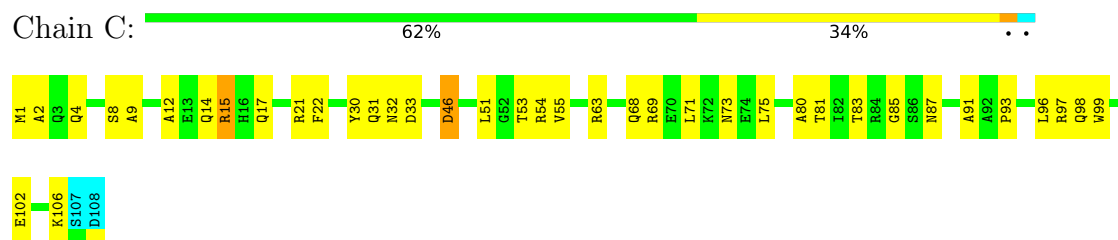
- Molecule 1: Trp operon repressor



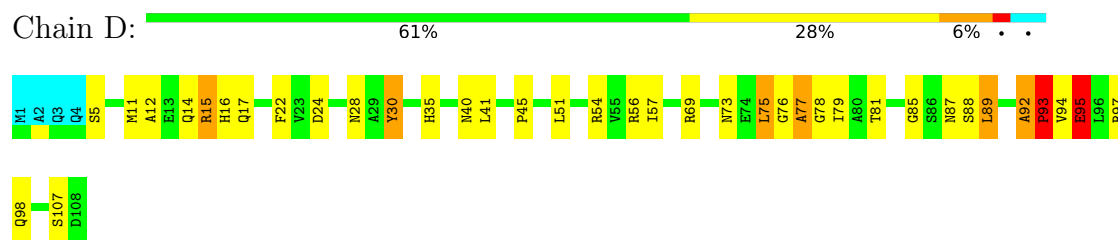
- Molecule 1: Trp operon repressor



- Molecule 1: Trp operon repressor

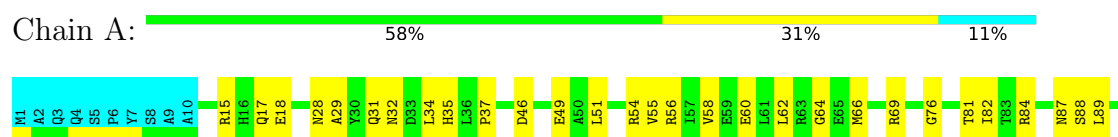


- Molecule 1: Trp operon repressor



4.2.6 Score per residue for model 6

- Molecule 1: Trp operon repressor





- Molecule 1: Trp operon repressor

Chain B: 55% 35% 8%



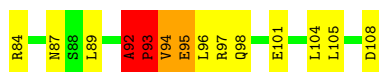
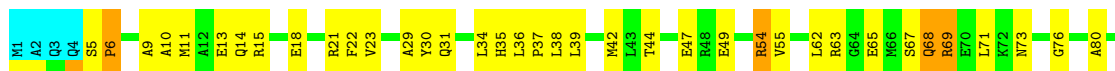
- Molecule 1: Trp operon repressor

Chain C: 63% 33% 2%



- Molecule 1: Trp operon repressor

Chain D: 49% 40% 6%



4.2.7 Score per residue for model 7

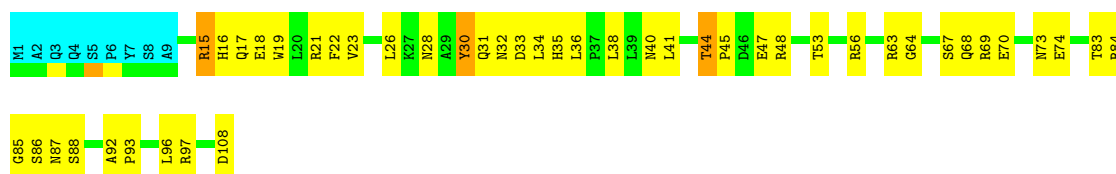
- Molecule 1: Trp operon repressor

Chain A: 57% 30% 11%



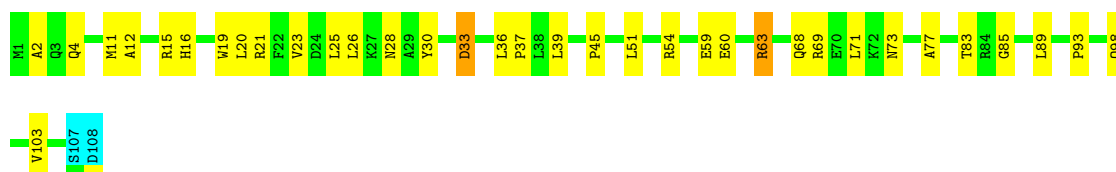
- Molecule 1: Trp operon repressor

Chain B: 50% 39% 8%



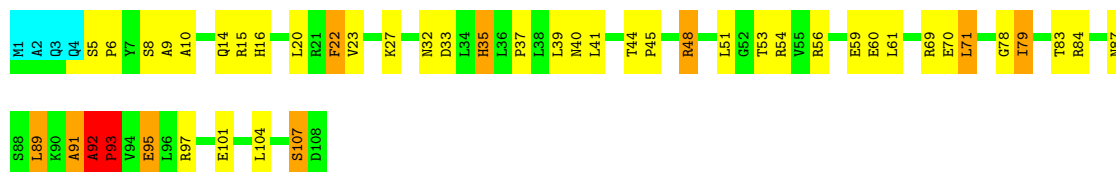
- Molecule 1: Trp operon repressor

Chain C: 66% 31% . .



- Molecule 1: Trp operon repressor

Chain D: 54% 32% 8% . .



4.2.8 Score per residue for model 8

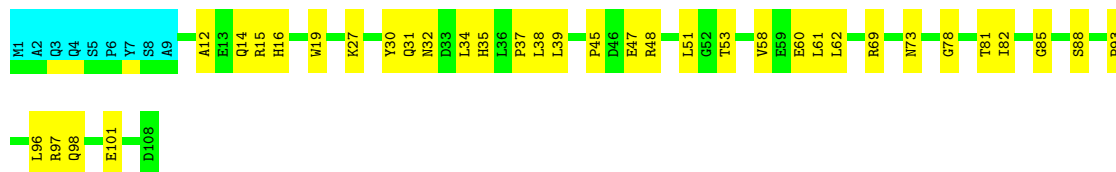
- Molecule 1: Trp operon repressor

Chain A: 66% 21% . 11%



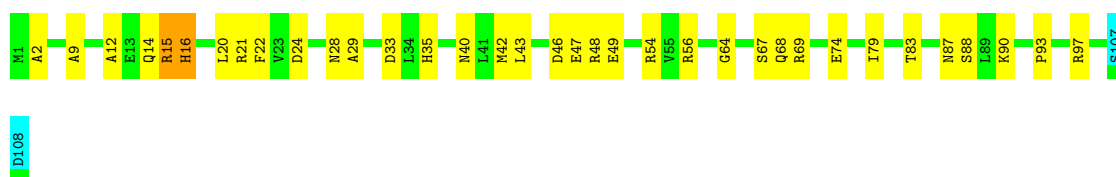
- Molecule 1: Trp operon repressor

Chain B: 59% 32% 8%



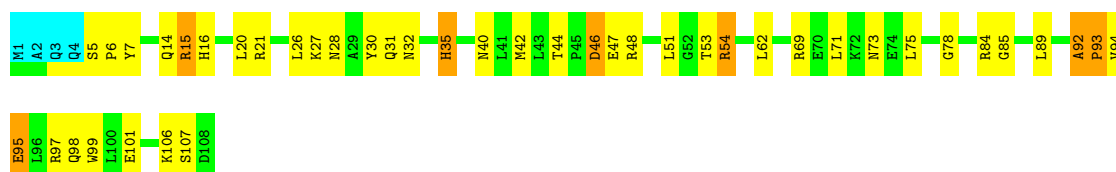
- Molecule 1: Trp operon repressor

Chain C: 66% 31% . .



- Molecule 1: Trp operon repressor

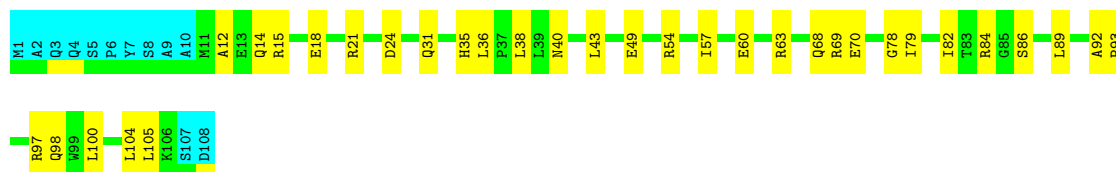
Chain D: 56% 33% 6%



4.2.9 Score per residue for model 9

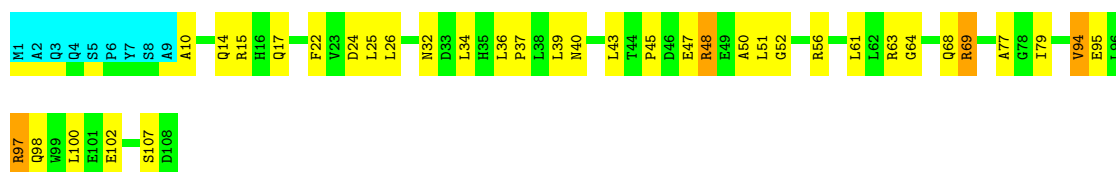
- Molecule 1: Trp operon repressor

Chain A: 58% 31% 11%



- Molecule 1: Trp operon repressor

Chain B: 58% 30% 8%

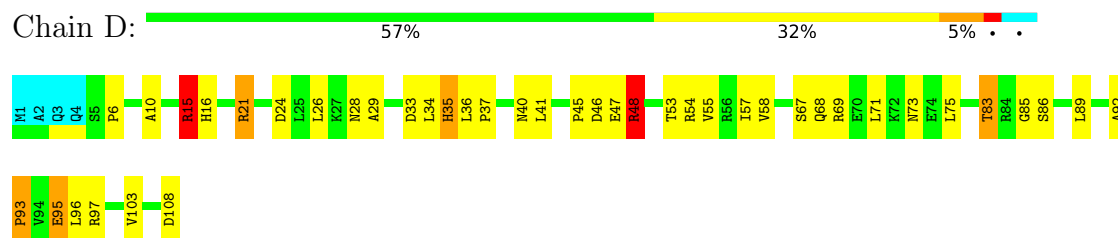


- Molecule 1: Trp operon repressor

Chain C: 65% 29% 5%

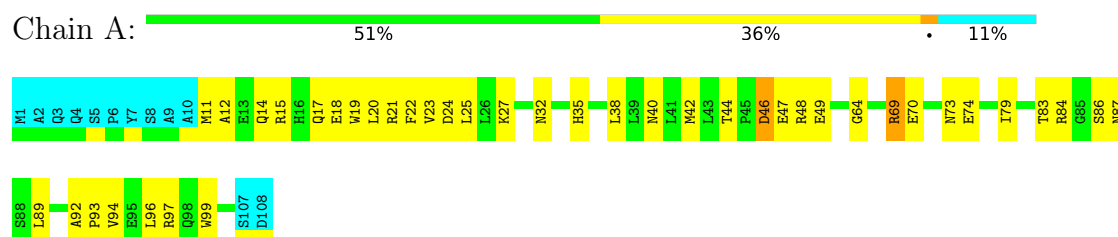


- Molecule 1: Trp operon repressor

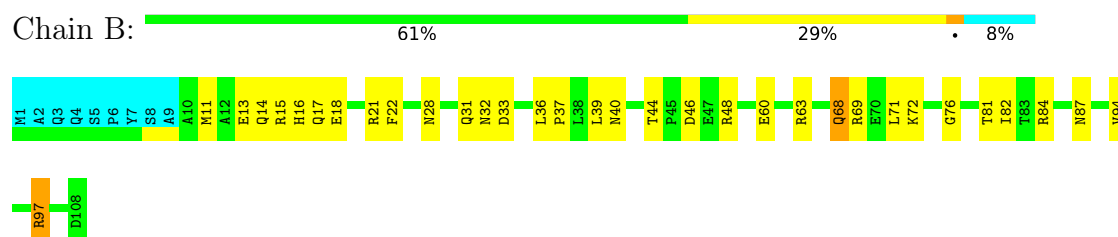


4.2.10 Score per residue for model 10

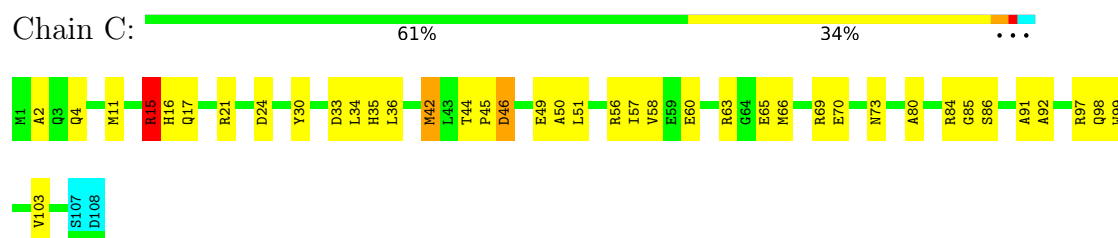
- Molecule 1: Trp operon repressor



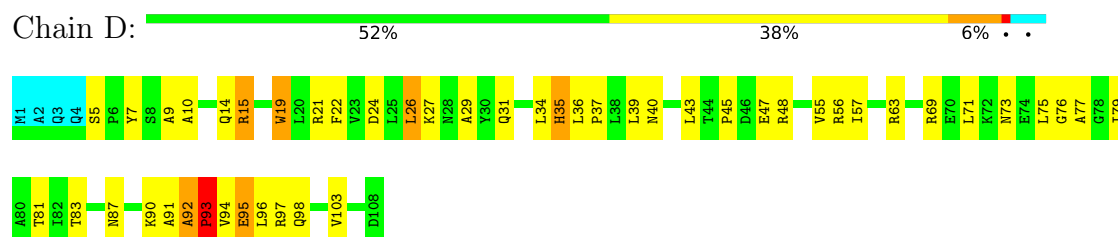
- Molecule 1: Trp operon repressor



- Molecule 1: Trp operon repressor

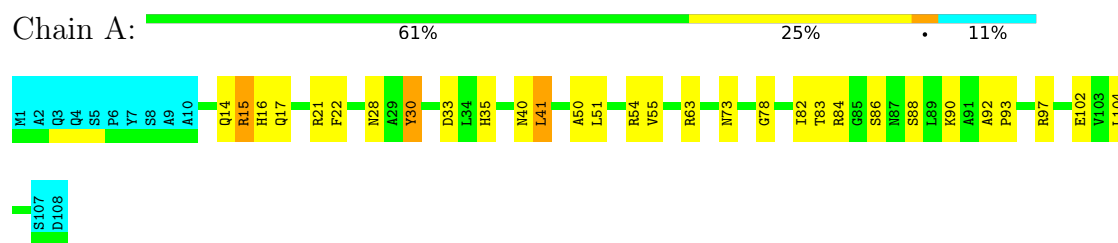


- Molecule 1: Trp operon repressor

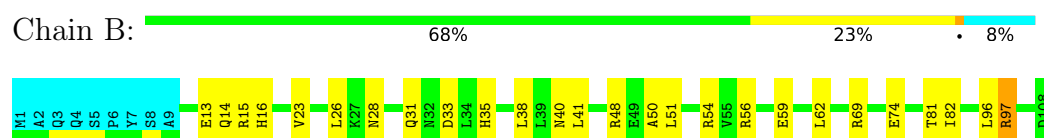


4.2.11 Score per residue for model 11

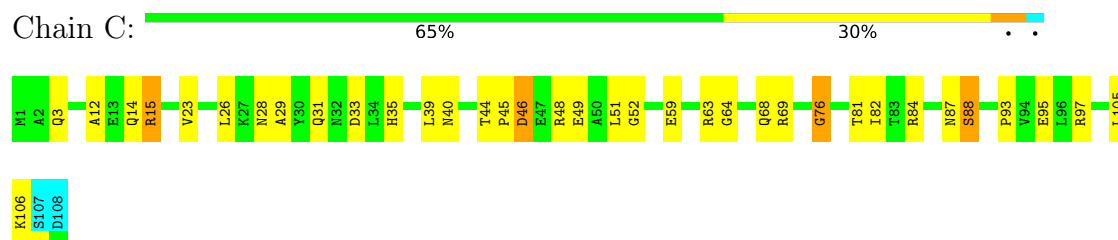
- Molecule 1: Trp operon repressor



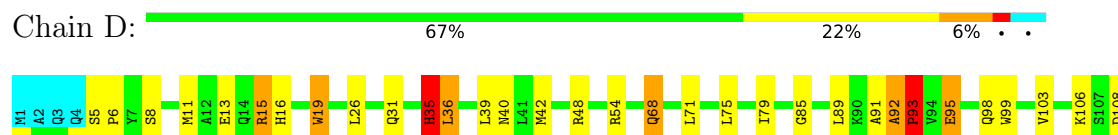
- Molecule 1: Trp operon repressor



- Molecule 1: Trp operon repressor

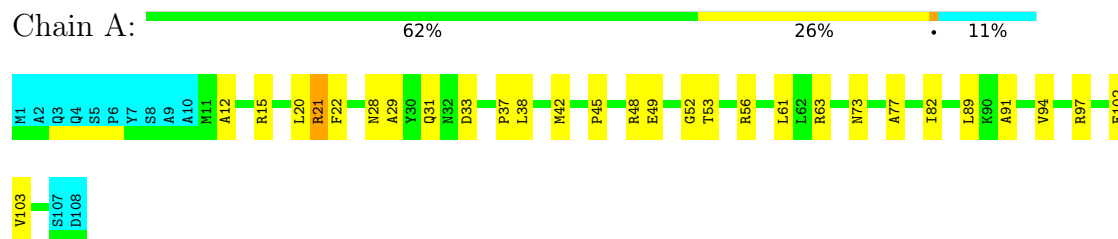


- Molecule 1: Trp operon repressor

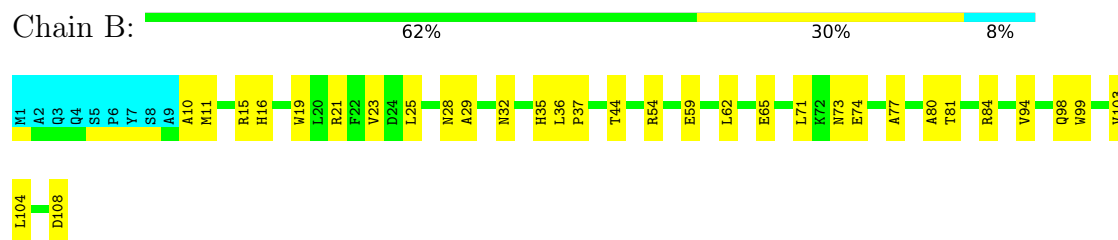


4.2.12 Score per residue for model 12

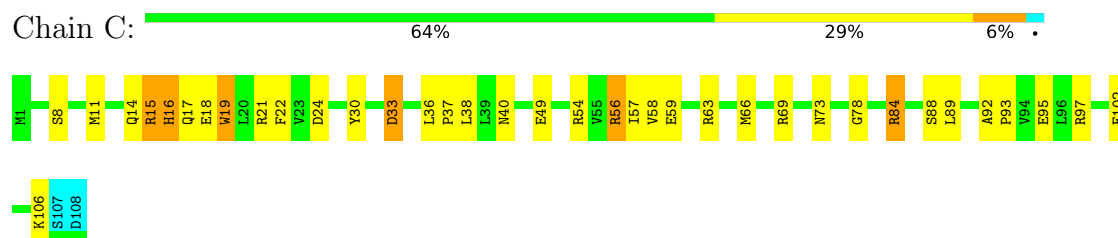
- Molecule 1: Trp operon repressor



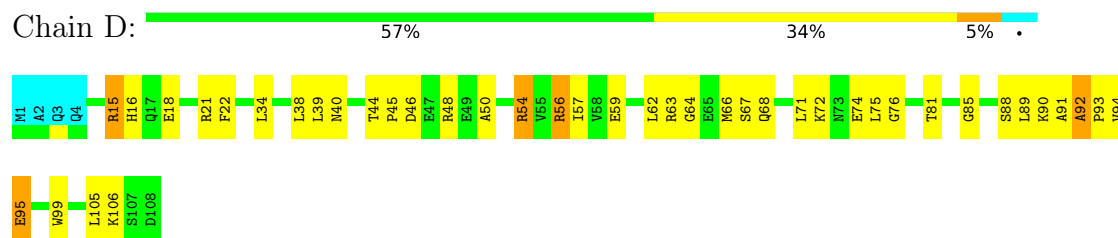
- Molecule 1: Trp operon repressor



- Molecule 1: Trp operon repressor

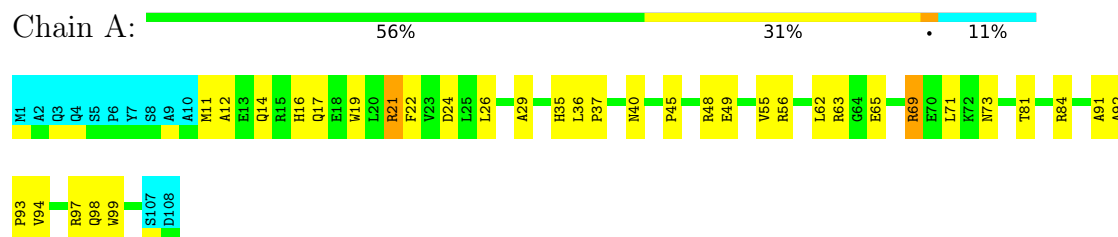


- Molecule 1: Trp operon repressor

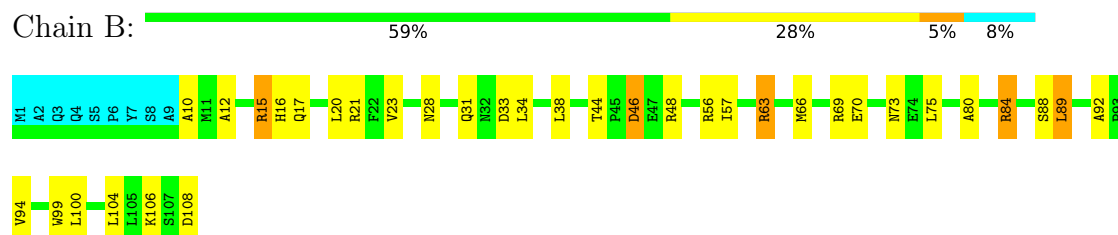


4.2.13 Score per residue for model 13

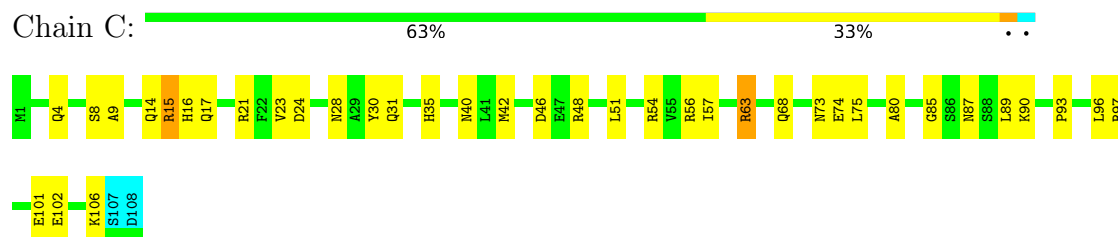
- Molecule 1: Trp operon repressor



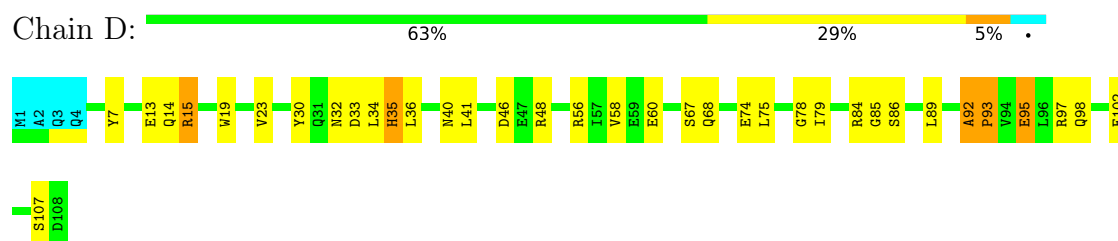
- Molecule 1: Trp operon repressor



- Molecule 1: Trp operon repressor

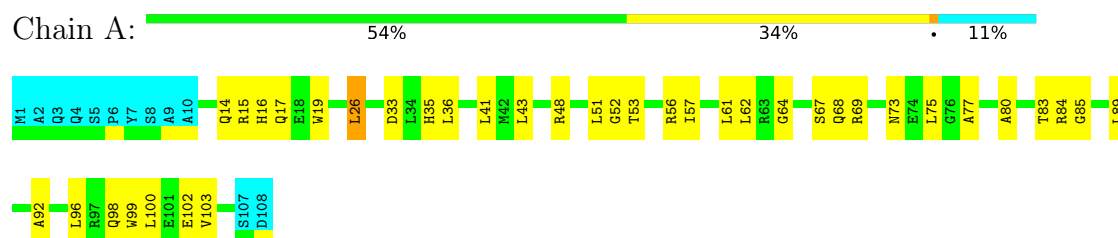


- Molecule 1: Trp operon repressor

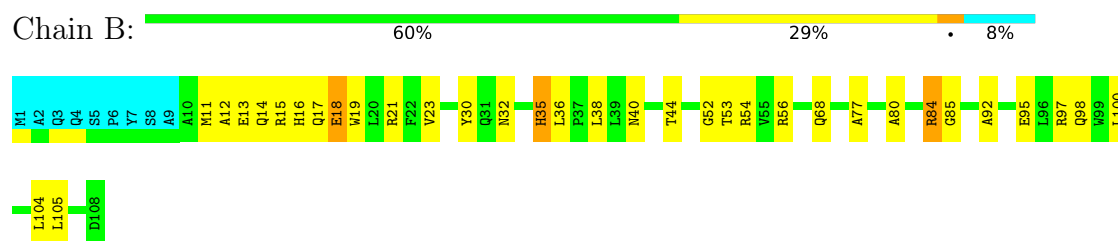


4.2.14 Score per residue for model 14

- Molecule 1: Trp operon repressor



- Molecule 1: Trp operon repressor



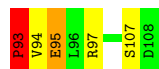
- Molecule 1: Trp operon repressor





- Molecule 1: Trp operon repressor

Chain D: 62% 29%



4.2.15 Score per residue for model 15

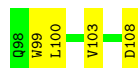
- Molecule 1: Trp operon repressor

Chain A: 58% 29% 11%



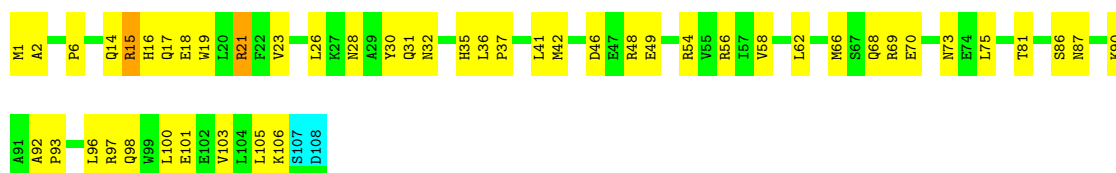
- Molecule 1: Trp operon repressor

Chain B: 57% 31% 8%



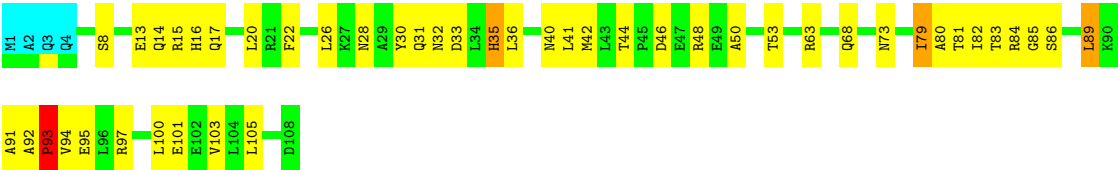
- Molecule 1: Trp operon repressor

Chain C: 54% 43%



- Molecule 1: Trp operon repressor

Chain D: 54% 39%



5 Refinement protocol and experimental data overview

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

Of the 15 calculated structures, 15 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
GROMACS	structure calculation	4.6.5
GROMACS	refinement	4.6.5

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	725
Number of shifts mapped to atoms	725
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	11%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.55±0.01	0±0/791 (0.0± 0.0%)	2.41±0.07	44±7/1068 (4.2± 0.6%)
1	B	0.55±0.01	0±0/810 (0.0± 0.0%)	2.42±0.07	50±9/1091 (4.6± 0.8%)
1	C	0.55±0.00	0±0/865 (0.0± 0.0%)	2.41±0.06	53±10/1169 (4.5± 0.8%)
1	D	0.55±0.01	0±0/848 (0.0± 0.0%)	2.40±0.07	49±7/1144 (4.2± 0.6%)
All	All	0.55	0/49710 (0.0%)	2.41	2939/67080 (4.4%)

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	2.3±1.4
1	B	0.0±0.0	2.8±1.0
1	C	0.0±0.0	2.1±1.2
1	D	0.0±0.0	5.3±1.9
All	All	0	187

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	73	ASN	OD1-CG-ND2	-12.51	110.09	122.60	6	4
1	B	68	GLN	OE1-CD-NE2	-11.77	110.83	122.60	10	5
1	B	40	ASN	OD1-CG-ND2	-11.63	110.97	122.60	2	4
1	B	69	ARG	NE-CZ-NH2	11.26	129.33	119.20	7	4
1	B	33	ASP	CA-CB-CG	11.01	123.61	112.60	7	2
1	A	28	ASN	OD1-CG-ND2	-10.91	111.69	122.60	6	4
1	D	21	ARG	NE-CZ-NH2	10.83	128.95	119.20	9	2
1	A	51	LEU	CA-C-N	10.61	131.72	119.94	6	3
1	A	51	LEU	C-N-CA	10.61	131.72	119.94	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	33	ASP	CA-CB-CG	10.59	123.19	112.60	7	4
1	A	73	ASN	OD1-CG-ND2	-10.54	112.06	122.60	12	4
1	A	14	GLN	OE1-CD-NE2	-10.53	112.07	122.60	14	7
1	C	14	GLN	OE1-CD-NE2	-10.49	112.11	122.60	3	5
1	A	93	PRO	N-CA-CB	10.44	112.55	103.36	10	4
1	C	21	ARG	NE-CZ-NH2	10.37	128.53	119.20	14	3
1	C	97	ARG	NE-CZ-NH2	10.35	128.52	119.20	10	9
1	D	97	ARG	NE-CZ-NH1	-10.34	111.17	121.50	13	3
1	D	48	ARG	CA-C-N	10.19	134.76	120.29	4	3
1	D	48	ARG	C-N-CA	10.19	134.76	120.29	4	3
1	B	28	ASN	OD1-CG-ND2	-10.18	112.42	122.60	7	4
1	A	87	ASN	CA-CB-CG	10.08	122.68	112.60	1	2
1	C	46	ASP	CA-CB-CG	10.07	122.67	112.60	11	6
1	C	62	LEU	CA-C-N	10.01	134.50	120.29	15	3
1	C	62	LEU	C-N-CA	10.01	134.50	120.29	15	3
1	B	71	LEU	CA-C-O	9.99	131.31	120.82	15	1
1	D	48	ARG	NE-CZ-NH1	9.98	131.48	121.50	8	3
1	B	87	ASN	CA-CB-CG	9.97	122.57	112.60	2	5
1	D	33	ASP	CA-CB-CG	9.89	122.49	112.60	15	2
1	B	84	ARG	CA-C-N	9.83	131.04	120.03	5	3
1	B	84	ARG	C-N-CA	9.83	131.04	120.03	5	3
1	A	69	ARG	NE-CZ-NH1	-9.79	111.71	121.50	13	4
1	A	78	GLY	O-C-N	9.73	131.36	122.99	11	1
1	C	36	LEU	CA-C-N	9.63	130.30	119.32	9	5
1	C	36	LEU	C-N-CA	9.63	130.30	119.32	9	5
1	A	24	ASP	CA-CB-CG	9.58	122.18	112.60	13	3
1	D	97	ARG	NE-CZ-NH2	9.56	127.81	119.20	15	8
1	B	98	GLN	OE1-CD-NE2	-9.55	113.05	122.60	14	4
1	A	17	GLN	OE1-CD-NE2	-9.54	113.06	122.60	4	1
1	B	15	ARG	NE-CZ-NH2	9.52	127.77	119.20	14	6
1	D	87	ASN	OD1-CG-ND2	-9.51	113.09	122.60	7	3
1	A	48	ARG	NE-CZ-NH1	9.49	130.99	121.50	14	3
1	B	108	ASP	CA-CB-CG	9.46	122.06	112.60	7	8
1	D	98	GLN	OE1-CD-NE2	-9.40	113.20	122.60	13	5
1	C	3	GLN	OE1-CD-NE2	-9.37	113.23	122.60	14	3
1	C	40	ASN	OD1-CG-ND2	-9.36	113.24	122.60	11	4
1	C	4	GLN	OE1-CD-NE2	-9.35	113.25	122.60	14	5
1	C	85	GLY	CA-C-O	-9.33	115.79	122.23	14	4
1	C	80	ALA	N-CA-C	9.32	121.13	110.97	14	1
1	D	108	ASP	CA-CB-CG	9.23	121.83	112.60	6	3
1	B	21	ARG	NE-CZ-NH1	9.23	130.73	121.50	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	48	ARG	CD-NE-CZ	9.19	137.26	124.40	7	2
1	C	21	ARG	NE-CZ-NH1	9.18	130.68	121.50	7	7
1	A	40	ASN	CA-CB-CG	9.17	121.77	112.60	3	3
1	D	28	ASN	CA-CB-CG	-9.17	103.43	112.60	9	5
1	A	15	ARG	NE-CZ-NH1	9.14	130.64	121.50	9	3
1	A	56	ARG	NE-CZ-NH1	9.13	130.63	121.50	12	1
1	B	32	ASN	OD1-CG-ND2	-9.13	113.47	122.60	2	6
1	D	97	ARG	CA-C-O	-9.11	110.79	120.63	15	4
1	C	102	GLU	CA-C-N	9.10	131.82	120.72	12	3
1	C	102	GLU	C-N-CA	9.10	131.82	120.72	12	3
1	A	97	ARG	NE-CZ-NH2	9.09	127.38	119.20	3	5
1	C	79	ILE	CA-C-O	-9.07	111.51	120.95	8	3
1	C	63	ARG	NE-CZ-NH2	9.05	127.35	119.20	7	7
1	B	51	LEU	N-CA-C	9.04	121.13	111.28	3	3
1	D	68	GLN	OE1-CD-NE2	-9.03	113.58	122.60	12	5
1	D	15	ARG	NE-CZ-NH2	9.00	127.30	119.20	14	2
1	A	94	VAL	O-C-N	8.98	130.59	121.87	7	3
1	C	73	ASN	OD1-CG-ND2	-8.97	113.63	122.60	10	6
1	D	48	ARG	NH1-CZ-NH2	-8.95	107.67	119.30	8	3
1	D	65	GLU	N-CA-C	-8.93	100.81	112.68	3	1
1	C	88	SER	CA-C-O	-8.90	111.71	121.94	9	2
1	B	23	VAL	CA-C-N	8.89	132.00	120.44	7	2
1	B	23	VAL	C-N-CA	8.89	132.00	120.44	7	2
1	B	80	ALA	N-CA-C	8.88	121.86	111.02	1	1
1	A	19	TRP	O-C-N	-8.87	112.93	122.07	4	2
1	A	54	ARG	NE-CZ-NH1	8.84	130.34	121.50	9	4
1	C	63	ARG	NE-CZ-NH1	8.82	130.32	121.50	3	3
1	A	21	ARG	NE-CZ-NH2	8.80	127.12	119.20	7	5
1	D	58	VAL	CA-CB-CG1	8.77	125.30	110.40	9	1
1	C	87	ASN	OD1-CG-ND2	-8.75	113.85	122.60	9	6
1	D	69	ARG	NE-CZ-NH2	-8.74	111.33	119.20	1	4
1	B	93	PRO	N-CA-CB	8.73	111.05	103.19	6	4
1	D	44	THR	CA-C-N	8.71	129.25	119.32	8	5
1	D	44	THR	C-N-CA	8.71	129.25	119.32	8	5
1	A	78	GLY	CA-C-N	8.71	131.53	120.56	4	3
1	A	78	GLY	C-N-CA	8.71	131.53	120.56	4	3
1	D	23	VAL	N-CA-CB	8.68	122.34	110.54	6	1
1	B	30	TYR	CA-C-O	-8.66	111.37	120.55	14	1
1	C	73	ASN	CA-CB-CG	8.63	121.23	112.60	10	2
1	A	98	GLN	OE1-CD-NE2	-8.62	113.98	122.60	14	6
1	C	69	ARG	NE-CZ-NH1	8.62	130.12	121.50	2	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	17	GLN	OE1-CD-NE2	-8.61	113.99	122.60	15	4
1	D	13	GLU	CA-C-O	8.57	130.07	120.90	6	2
1	A	92	ALA	CA-C-N	8.56	128.60	119.78	6	7
1	A	92	ALA	C-N-CA	8.56	128.60	119.78	6	7
1	B	78	GLY	CA-C-N	8.53	131.60	120.60	4	4
1	B	78	GLY	C-N-CA	8.53	131.60	120.60	4	4
1	A	46	ASP	CA-C-N	8.50	131.67	120.28	5	1
1	A	46	ASP	C-N-CA	8.50	131.67	120.28	5	1
1	C	98	GLN	OE1-CD-NE2	-8.50	114.10	122.60	15	2
1	D	32	ASN	OD1-CG-ND2	-8.49	114.11	122.60	7	4
1	B	17	GLN	OE1-CD-NE2	-8.46	114.14	122.60	9	6
1	B	68	GLN	CA-C-N	8.46	131.44	120.44	14	2
1	B	68	GLN	C-N-CA	8.46	131.44	120.44	14	2
1	D	54	ARG	NE-CZ-NH2	-8.45	111.59	119.20	1	4
1	C	35	HIS	CB-CG-CD2	-8.44	120.22	131.20	3	5
1	C	84	ARG	NE-CZ-NH1	8.42	129.92	121.50	14	1
1	D	5	SER	CA-C-N	8.41	128.10	119.19	3	5
1	D	5	SER	C-N-CA	8.41	128.10	119.19	3	5
1	C	69	ARG	NE-CZ-NH2	-8.41	111.63	119.20	2	1
1	A	41	LEU	N-CA-C	8.40	120.52	111.36	4	1
1	B	101	GLU	CA-C-O	-8.38	111.66	120.55	6	1
1	A	15	ARG	NE-CZ-NH2	8.38	126.74	119.20	5	4
1	D	63	ARG	NH1-CZ-NH2	-8.37	108.41	119.30	10	6
1	A	21	ARG	CD-NE-CZ	8.37	136.12	124.40	7	2
1	D	69	ARG	NE-CZ-NH1	8.37	129.87	121.50	7	2
1	D	40	ASN	OD1-CG-ND2	-8.32	114.28	122.60	15	9
1	B	82	ILE	CA-C-N	8.32	131.26	120.44	8	4
1	B	82	ILE	C-N-CA	8.32	131.26	120.44	8	4
1	C	69	ARG	N-CA-C	8.31	119.97	111.07	10	1
1	B	23	VAL	CA-C-O	-8.31	112.36	121.17	1	1
1	B	46	ASP	CA-CB-CG	8.30	120.90	112.60	13	2
1	C	17	GLN	OE1-CD-NE2	-8.29	114.31	122.60	9	4
1	D	89	LEU	N-CA-C	8.29	122.36	111.75	2	3
1	C	58	VAL	CA-C-N	8.27	131.71	120.54	15	3
1	C	58	VAL	C-N-CA	8.27	131.71	120.54	15	3
1	D	93	PRO	CA-N-CD	-8.27	99.92	111.50	15	8
1	B	15	ARG	NH1-CZ-NH2	-8.26	108.57	119.30	7	3
1	C	13	GLU	CA-C-O	-8.26	109.22	119.38	14	1
1	B	16	HIS	CB-CG-CD2	-8.24	120.49	131.20	10	5
1	D	40	ASN	CA-CB-CG	8.20	120.80	112.60	3	8
1	D	22	PHE	CA-CB-CG	-8.19	105.61	113.80	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	84	ARG	NE-CZ-NH2	8.18	126.56	119.20	14	5
1	A	56	ARG	NE-CZ-NH2	8.17	126.56	119.20	13	3
1	B	35	HIS	CB-CG-CD2	-8.15	120.60	131.20	1	6
1	C	16	HIS	CA-CB-CG	8.15	121.95	113.80	10	4
1	C	5	SER	N-CA-C	8.15	117.51	108.14	6	1
1	A	33	ASP	CA-CB-CG	8.14	120.74	112.60	11	2
1	A	31	GLN	OE1-CD-NE2	-8.12	114.47	122.60	6	4
1	A	35	HIS	CB-CG-CD2	-8.11	120.65	131.20	9	5
1	D	83	THR	N-CA-C	8.11	123.34	112.88	4	3
1	C	22	PHE	N-CA-CB	8.08	122.10	109.82	3	1
1	A	63	ARG	NE-CZ-NH1	8.08	129.58	121.50	13	1
1	D	86	SER	N-CA-C	8.07	120.16	111.36	14	3
1	B	81	THR	CA-C-N	8.07	130.88	120.56	11	2
1	B	81	THR	C-N-CA	8.07	130.88	120.56	11	2
1	A	29	ALA	CA-C-O	-8.05	111.88	120.42	5	3
1	A	15	ARG	NH1-CZ-NH2	-8.05	108.83	119.30	9	4
1	C	24	ASP	CA-C-N	8.05	131.39	120.44	1	3
1	C	24	ASP	C-N-CA	8.05	131.39	120.44	1	3
1	B	21	ARG	NE-CZ-NH2	8.05	126.44	119.20	6	5
1	D	8	SER	CA-C-N	8.04	131.05	120.28	2	3
1	D	8	SER	C-N-CA	8.04	131.05	120.28	2	3
1	D	46	ASP	CA-CB-CG	8.03	120.63	112.60	8	2
1	B	54	ARG	NH1-CZ-NH2	-8.02	108.87	119.30	4	3
1	D	54	ARG	NH1-CZ-NH2	-8.01	108.89	119.30	6	3
1	C	11	MET	N-CA-C	8.00	121.10	111.82	12	1
1	D	84	ARG	NE-CZ-NH2	8.00	126.40	119.20	2	1
1	A	97	ARG	NE-CZ-NH1	-8.00	113.50	121.50	10	3
1	B	92	ALA	CA-C-N	7.99	127.94	120.03	13	3
1	B	92	ALA	C-N-CA	7.99	127.94	120.03	13	3
1	C	58	VAL	N-CA-C	7.99	118.09	110.42	1	2
1	B	73	ASN	OD1-CG-ND2	-7.99	114.61	122.60	6	5
1	D	97	ARG	N-CA-C	7.96	120.97	111.33	14	2
1	B	28	ASN	CA-CB-CG	-7.96	104.64	112.60	11	7
1	C	87	ASN	CA-CB-CG	7.96	120.56	112.60	2	2
1	C	103	VAL	CA-CB-CG2	7.96	123.93	110.40	15	1
1	B	62	LEU	N-CA-C	7.96	122.76	112.89	6	3
1	D	34	LEU	CA-C-N	7.94	130.76	120.44	10	7
1	D	34	LEU	C-N-CA	7.94	130.76	120.44	10	7
1	C	19	TRP	CE2-CD2-CE3	-7.93	110.87	118.80	12	1
1	B	73	ASN	CA-CB-CG	7.93	120.53	112.60	13	4
1	C	18	GLU	CA-C-N	7.92	130.90	120.28	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	18	GLU	C-N-CA	7.92	130.90	120.28	14	1
1	D	21	ARG	CD-NE-CZ	7.91	135.47	124.40	8	1
1	A	49	GLU	CA-C-N	7.91	130.88	120.28	4	5
1	A	49	GLU	C-N-CA	7.91	130.88	120.28	4	5
1	A	32	ASN	OD1-CG-ND2	-7.91	114.69	122.60	3	3
1	C	93	PRO	N-CA-CB	7.90	110.23	103.35	11	6
1	D	21	ARG	NH1-CZ-NH2	-7.88	109.06	119.30	9	1
1	A	69	ARG	NE-CZ-NH2	7.88	126.29	119.20	13	7
1	D	35	HIS	CB-CG-CD2	-7.87	120.97	131.20	14	7
1	C	97	ARG	NH1-CZ-NH2	-7.87	109.07	119.30	15	1
1	D	55	VAL	CB-CA-C	-7.87	101.52	112.14	2	1
1	A	54	ARG	NH1-CZ-NH2	-7.86	109.08	119.30	9	4
1	C	68	GLN	OE1-CD-NE2	-7.85	114.75	122.60	14	7
1	D	75	LEU	N-CA-C	-7.84	102.68	111.14	9	1
1	A	21	ARG	NE-CZ-NH1	7.83	129.34	121.50	4	4
1	D	95	GLU	CA-C-N	7.81	131.06	120.44	11	3
1	D	95	GLU	C-N-CA	7.81	131.06	120.44	11	3
1	D	31	GLN	OE1-CD-NE2	-7.80	114.80	122.60	11	3
1	B	43	LEU	O-C-N	-7.80	113.84	123.36	9	1
1	D	14	GLN	OE1-CD-NE2	-7.80	114.80	122.60	6	5
1	A	40	ASN	CA-C-N	7.80	133.91	120.58	11	2
1	A	40	ASN	C-N-CA	7.80	133.91	120.58	11	2
1	A	63	ARG	NE-CZ-NH2	7.80	126.22	119.20	11	5
1	C	56	ARG	CA-C-O	-7.79	112.16	120.42	15	4
1	A	91	ALA	CA-C-N	7.77	131.09	120.67	13	2
1	A	91	ALA	C-N-CA	7.77	131.09	120.67	13	2
1	D	63	ARG	NE-CZ-NH2	7.77	126.19	119.20	10	3
1	B	77	ALA	N-CA-C	7.76	121.73	107.99	6	4
1	D	93	PRO	CB-CA-C	7.76	124.36	111.56	3	2
1	A	83	THR	CA-C-N	7.76	130.67	120.28	5	1
1	A	83	THR	C-N-CA	7.76	130.67	120.28	5	1
1	C	89	LEU	N-CA-C	7.75	120.71	111.33	1	4
1	C	100	LEU	CA-C-N	7.74	132.08	120.31	14	1
1	C	100	LEU	C-N-CA	7.74	132.08	120.31	14	1
1	C	33	ASP	N-CA-C	7.73	122.29	112.86	9	2
1	D	84	ARG	NE-CZ-NH1	7.73	129.23	121.50	4	4
1	C	83	THR	N-CA-C	7.72	122.85	112.88	8	3
1	D	24	ASP	N-CA-C	7.72	120.78	111.82	2	3
1	B	99	TRP	CA-C-N	7.72	131.39	120.28	13	1
1	B	99	TRP	C-N-CA	7.72	131.39	120.28	13	1
1	C	34	LEU	CA-C-N	7.71	130.95	120.38	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	34	LEU	C-N-CA	7.71	130.95	120.38	10	1
1	B	74	GLU	N-CA-C	7.70	120.56	111.71	15	1
1	A	68	GLN	OE1-CD-NE2	-7.68	114.92	122.60	7	6
1	B	97	ARG	CD-NE-CZ	7.68	135.16	124.40	3	1
1	D	9	ALA	CA-C-N	7.68	130.89	120.44	7	3
1	D	9	ALA	C-N-CA	7.68	130.89	120.44	7	3
1	D	56	ARG	NH1-CZ-NH2	-7.68	109.32	119.30	10	5
1	B	96	LEU	CA-C-N	7.68	130.90	120.38	11	2
1	B	96	LEU	C-N-CA	7.68	130.90	120.38	11	2
1	B	69	ARG	NE-CZ-NH1	-7.68	113.82	121.50	13	1
1	A	73	ASN	CA-CB-CG	7.67	120.27	112.60	1	1
1	C	48	ARG	NE-CZ-NH1	7.66	129.16	121.50	8	1
1	C	65	GLU	N-CA-C	7.66	121.88	112.54	1	1
1	B	57	ILE	CA-CB-CG1	7.65	123.40	110.40	2	1
1	B	47	GLU	N-CA-C	7.64	119.61	111.28	2	1
1	A	73	ASN	N-CA-C	7.64	119.61	111.28	2	1
1	B	56	ARG	CD-NE-CZ	7.64	135.09	124.40	7	2
1	D	101	GLU	CA-C-O	-7.64	111.47	120.10	7	1
1	B	48	ARG	NE-CZ-NH1	7.63	129.13	121.50	9	4
1	C	64	GLY	CA-C-O	-7.63	110.55	119.02	8	2
1	D	103	VAL	CA-C-O	7.63	125.70	119.29	11	2
1	C	68	GLN	CA-C-N	7.62	130.70	120.65	7	3
1	C	68	GLN	C-N-CA	7.62	130.70	120.65	7	3
1	D	71	LEU	N-CA-C	7.61	120.53	111.33	14	1
1	D	6	PRO	N-CA-CB	7.60	110.80	103.51	8	5
1	C	78	GLY	CA-C-O	-7.59	110.69	119.65	6	1
1	B	32	ASN	CA-CB-CG	7.59	120.19	112.60	7	4
1	A	53	THR	N-CA-C	7.57	119.61	111.36	12	1
1	C	15	ARG	NE-CZ-NH1	7.56	129.06	121.50	10	5
1	A	36	LEU	CA-C-N	7.56	127.94	119.32	13	4
1	A	36	LEU	C-N-CA	7.56	127.94	119.32	13	4
1	D	42	MET	N-CA-C	7.56	119.60	111.36	6	1
1	C	3	GLN	N-CA-C	7.56	121.97	109.95	2	1
1	B	16	HIS	ND1-CG-CD2	7.56	113.66	106.10	10	2
1	A	81	THR	CA-C-N	7.56	129.94	120.72	6	1
1	A	81	THR	C-N-CA	7.56	129.94	120.72	6	1
1	D	53	THR	O-C-N	-7.55	114.30	122.07	8	2
1	A	102	GLU	CA-C-N	7.54	129.93	120.72	14	3
1	A	102	GLU	C-N-CA	7.54	129.93	120.72	14	3
1	D	54	ARG	N-CA-C	7.54	121.58	112.38	12	2
1	D	92	ALA	CA-C-N	7.54	129.26	119.84	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	92	ALA	C-N-CA	7.54	129.26	119.84	14	2
1	A	16	HIS	CB-CG-CD2	-7.53	121.41	131.20	13	6
1	B	22	PHE	N-CA-C	7.53	119.49	111.28	10	1
1	D	16	HIS	CB-CG-CD2	-7.53	121.42	131.20	7	6
1	C	39	LEU	N-CA-C	7.52	121.38	111.75	7	1
1	D	11	MET	CA-C-O	-7.52	112.96	120.70	11	1
1	C	28	ASN	OD1-CG-ND2	-7.52	115.08	122.60	4	6
1	B	58	VAL	CA-CB-CG1	7.52	123.18	110.40	3	2
1	D	106	LYS	CA-C-N	7.51	130.67	120.38	8	1
1	D	106	LYS	C-N-CA	7.51	130.67	120.38	8	1
1	A	38	LEU	CA-C-N	7.50	130.34	120.28	4	1
1	A	38	LEU	C-N-CA	7.50	130.34	120.28	4	1
1	A	68	GLN	CA-C-N	7.49	131.07	120.28	4	1
1	A	68	GLN	C-N-CA	7.49	131.07	120.28	4	1
1	C	42	MET	N-CA-C	7.49	121.68	112.54	15	3
1	D	93	PRO	CA-C-N	7.49	130.72	120.46	6	1
1	D	93	PRO	C-N-CA	7.49	130.72	120.46	6	1
1	D	54	ARG	CA-C-O	-7.48	111.64	120.10	8	3
1	A	56	ARG	CA-C-O	-7.48	112.62	120.55	3	1
1	B	97	ARG	CA-C-N	7.47	130.30	120.28	5	2
1	B	97	ARG	C-N-CA	7.47	130.30	120.28	5	2
1	D	56	ARG	NE-CZ-NH1	7.47	128.97	121.50	12	3
1	B	48	ARG	N-CA-C	7.47	119.42	111.28	15	1
1	C	35	HIS	CA-CB-CG	7.46	121.26	113.80	6	5
1	A	19	TRP	CB-CG-CD1	-7.45	115.72	126.90	3	2
1	C	63	ARG	NH1-CZ-NH2	-7.45	109.62	119.30	1	4
1	D	73	ASN	CA-CB-CG	7.45	120.05	112.60	9	5
1	B	14	GLN	CA-C-O	-7.45	112.66	120.55	8	2
1	B	35	HIS	N-CA-C	7.44	119.39	111.28	6	2
1	C	54	ARG	CD-NE-CZ	7.44	134.81	124.40	5	2
1	C	14	GLN	CA-C-N	7.44	130.11	120.44	8	4
1	C	14	GLN	C-N-CA	7.44	130.11	120.44	8	4
1	A	84	ARG	CD-NE-CZ	7.43	134.81	124.40	2	1
1	B	40	ASN	CB-CG-ND2	7.43	127.55	116.40	2	1
1	A	54	ARG	NE-CZ-NH2	-7.43	112.52	119.20	4	2
1	C	25	LEU	CA-C-O	-7.42	113.06	120.70	1	3
1	D	63	ARG	NE-CZ-NH1	7.42	128.91	121.50	15	2
1	C	88	SER	CA-C-N	7.41	130.54	120.38	11	3
1	C	88	SER	C-N-CA	7.41	130.54	120.38	11	3
1	C	56	ARG	NE-CZ-NH2	7.41	125.87	119.20	9	2
1	A	96	LEU	CA-C-O	-7.41	112.70	120.55	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	69	ARG	CA-C-N	7.38	130.48	120.44	8	1
1	D	69	ARG	C-N-CA	7.38	130.48	120.44	8	1
1	A	86	SER	N-CA-C	7.38	118.97	111.07	9	1
1	A	20	LEU	CA-C-N	7.38	130.47	120.44	3	3
1	A	20	LEU	C-N-CA	7.38	130.47	120.44	3	3
1	A	104	LEU	O-C-N	-7.37	113.32	122.24	4	1
1	D	24	ASP	CA-CB-CG	-7.36	105.24	112.60	4	2
1	A	19	TRP	CE2-CD2-CE3	-7.36	111.44	118.80	13	1
1	A	80	ALA	N-CA-C	7.35	120.16	111.71	14	1
1	C	78	GLY	O-C-N	7.33	130.61	122.54	6	2
1	B	56	ARG	NH1-CZ-NH2	-7.32	109.78	119.30	6	3
1	D	27	LYS	O-C-N	7.32	129.91	122.08	7	1
1	C	65	GLU	CB-CA-C	7.31	120.29	111.22	10	1
1	C	93	PRO	CA-C-N	7.30	129.91	120.56	6	5
1	C	93	PRO	C-N-CA	7.30	129.91	120.56	6	5
1	B	59	GLU	N-CA-C	7.30	119.32	111.36	11	3
1	D	67	SER	N-CA-C	7.30	121.41	109.94	4	5
1	B	12	ALA	CA-C-N	7.30	130.56	120.63	3	3
1	B	12	ALA	C-N-CA	7.30	130.56	120.63	3	3
1	C	52	GLY	CA-C-N	7.27	130.25	120.65	11	2
1	C	52	GLY	C-N-CA	7.27	130.25	120.65	11	2
1	B	38	LEU	N-CA-C	7.27	119.20	111.28	14	1
1	C	21	ARG	CA-C-O	-7.26	112.72	120.42	5	1
1	C	88	SER	N-CA-C	7.26	119.94	110.43	3	1
1	C	3	GLN	CA-C-O	-7.24	112.98	121.16	2	1
1	D	35	HIS	CA-CB-CG	7.24	121.04	113.80	9	5
1	A	12	ALA	CA-C-O	-7.23	111.93	120.10	13	3
1	D	37	PRO	CB-CA-C	-7.22	101.56	112.11	6	1
1	A	22	PHE	CA-CB-CG	-7.22	106.58	113.80	11	1
1	D	10	ALA	CA-C-O	7.22	128.26	120.24	6	1
1	B	56	ARG	CA-C-O	-7.22	112.90	120.55	13	1
1	B	26	LEU	N-CA-C	7.22	118.79	111.07	9	2
1	B	77	ALA	CA-C-N	7.22	127.89	120.60	14	2
1	B	77	ALA	C-N-CA	7.22	127.89	120.60	14	2
1	B	73	ASN	CA-C-N	7.21	132.14	120.60	13	1
1	B	73	ASN	C-N-CA	7.21	132.14	120.60	13	1
1	B	35	HIS	CA-C-O	-7.21	112.78	120.42	4	2
1	B	23	VAL	N-CA-C	7.21	117.31	110.53	12	2
1	C	23	VAL	CB-CA-C	7.21	120.92	111.70	13	2
1	A	89	LEU	CA-C-N	7.20	130.26	120.54	10	3
1	A	89	LEU	C-N-CA	7.20	130.26	120.54	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	94	VAL	CA-C-O	-7.20	113.54	121.17	1	2
1	C	35	HIS	N-CA-C	7.19	119.12	111.28	13	2
1	A	23	VAL	N-CA-C	7.19	117.95	110.62	8	1
1	A	44	THR	CA-C-N	7.18	127.51	119.32	7	3
1	A	44	THR	C-N-CA	7.18	127.51	119.32	7	3
1	C	54	ARG	CA-C-O	-7.18	110.55	119.38	8	2
1	C	55	VAL	CA-C-O	-7.18	113.58	121.05	5	4
1	B	14	GLN	OE1-CD-NE2	-7.17	115.43	122.60	1	6
1	C	18	GLU	O-C-N	7.16	129.71	122.12	12	2
1	B	54	ARG	N-CA-CB	7.15	121.24	110.22	6	1
1	D	37	PRO	N-CA-CB	7.15	111.10	103.52	6	3
1	D	56	ARG	CA-C-N	7.15	129.71	120.56	4	4
1	D	56	ARG	C-N-CA	7.15	129.71	120.56	4	4
1	D	87	ASN	O-C-N	7.14	129.25	122.18	2	1
1	A	24	ASP	CA-C-N	7.14	131.53	120.82	9	2
1	A	24	ASP	C-N-CA	7.14	131.53	120.82	9	2
1	A	30	TYR	CA-C-O	-7.14	112.98	120.55	7	1
1	A	46	ASP	CA-CB-CG	7.13	119.73	112.60	3	5
1	A	33	ASP	CA-C-N	7.13	133.54	122.49	12	1
1	A	33	ASP	C-N-CA	7.13	133.54	122.49	12	1
1	C	9	ALA	N-CA-C	7.12	121.56	113.01	3	2
1	B	62	LEU	CA-C-N	7.11	130.03	120.65	11	2
1	B	62	LEU	C-N-CA	7.11	130.03	120.65	11	2
1	B	54	ARG	NE-CZ-NH2	7.11	125.60	119.20	4	2
1	B	10	ALA	N-CA-CB	7.11	120.32	110.01	13	1
1	C	10	ALA	CA-C-O	-7.10	113.03	120.55	1	1
1	A	21	ARG	NH1-CZ-NH2	-7.09	110.08	119.30	4	5
1	B	76	GLY	CA-C-N	7.08	132.28	122.79	10	2
1	B	76	GLY	C-N-CA	7.08	132.28	122.79	10	2
1	C	27	LYS	CA-C-N	7.08	129.77	120.28	6	1
1	C	27	LYS	C-N-CA	7.08	129.77	120.28	6	1
1	D	16	HIS	ND1-CG-CD2	7.08	113.18	106.10	1	7
1	C	6	PRO	N-CA-C	7.08	124.07	113.81	2	1
1	B	100	LEU	CA-C-O	-7.07	111.83	119.97	14	2
1	A	16	HIS	N-CA-C	7.06	119.06	111.36	8	2
1	D	38	LEU	CA-C-O	-7.06	112.40	120.24	12	2
1	C	14	GLN	O-C-N	-7.06	114.64	122.12	13	2
1	B	38	LEU	CA-C-O	-7.05	113.43	120.70	7	3
1	C	53	THR	O-C-N	-7.05	114.76	122.09	14	1
1	C	39	LEU	CA-C-N	7.04	131.01	120.31	1	2
1	C	39	LEU	C-N-CA	7.04	131.01	120.31	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	84	ARG	NH1-CZ-NH2	-7.03	110.17	119.30	10	2
1	C	28	ASN	CA-CB-CG	-7.03	105.57	112.60	7	1
1	D	104	LEU	CA-C-O	-7.02	111.28	119.78	7	2
1	B	54	ARG	CA-C-O	-7.02	113.11	120.55	12	2
1	B	65	GLU	CA-CB-CG	7.01	128.13	114.10	15	1
1	C	11	MET	CA-C-N	7.00	129.66	120.28	4	2
1	C	11	MET	C-N-CA	7.00	129.66	120.28	4	2
1	D	32	ASN	CA-CB-CG	7.00	119.60	112.60	8	1
1	B	78	GLY	O-C-N	-6.99	117.25	122.71	5	1
1	A	35	HIS	ND1-CE1-NE2	6.99	115.39	108.40	1	3
1	C	101	GLU	CA-C-N	6.98	129.52	120.44	6	2
1	C	101	GLU	C-N-CA	6.98	129.52	120.44	6	2
1	A	19	TRP	CA-C-O	6.98	128.15	120.82	4	2
1	B	44	THR	CA-CB-OG1	6.98	120.08	109.60	12	4
1	D	73	ASN	CB-CG-ND2	6.97	126.86	116.40	4	1
1	A	99	TRP	CE2-CD2-CE3	-6.97	111.83	118.80	13	2
1	B	16	HIS	ND1-CE1-NE2	6.97	115.37	108.40	8	1
1	B	97	ARG	N-CA-CB	-6.97	99.88	110.12	8	1
1	B	102	GLU	N-CA-C	6.96	121.04	112.54	9	1
1	C	104	LEU	N-CA-C	6.96	121.77	113.28	2	1
1	C	16	HIS	ND1-CG-CD2	6.96	113.06	106.10	13	4
1	B	22	PHE	CA-C-N	6.95	129.99	120.46	5	3
1	B	22	PHE	C-N-CA	6.95	129.99	120.46	5	3
1	A	47	GLU	CA-C-N	6.95	129.89	120.44	5	2
1	A	47	GLU	C-N-CA	6.95	129.89	120.44	5	2
1	D	59	GLU	N-CA-C	6.95	119.45	111.11	12	1
1	B	97	ARG	NH1-CZ-NH2	-6.94	110.28	119.30	6	2
1	B	30	TYR	N-CA-C	6.94	119.73	111.33	7	2
1	D	26	LEU	CA-C-O	-6.94	113.53	120.82	11	4
1	A	87	ASN	OD1-CG-ND2	-6.94	115.66	122.60	4	4
1	B	83	THR	CA-C-N	6.93	130.50	120.38	7	2
1	B	83	THR	C-N-CA	6.93	130.50	120.38	7	2
1	C	97	ARG	NE-CZ-NH1	-6.93	114.57	121.50	10	3
1	A	92	ALA	O-C-N	6.93	128.21	121.28	13	1
1	D	73	ASN	CA-C-N	6.92	129.44	120.44	2	1
1	D	73	ASN	C-N-CA	6.92	129.44	120.44	2	1
1	A	49	GLU	O-C-N	-6.92	114.79	122.12	4	2
1	A	33	ASP	N-CA-C	6.92	121.47	113.38	11	1
1	D	65	GLU	O-C-N	6.92	129.43	122.10	14	1
1	C	15	ARG	CA-C-O	6.92	127.92	119.97	11	3
1	C	56	ARG	NE-CZ-NH1	6.92	128.42	121.50	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	56	ARG	CA-C-N	6.91	129.40	120.56	6	1
1	C	56	ARG	C-N-CA	6.91	129.40	120.56	6	1
1	D	81	THR	CA-C-N	6.91	131.45	121.02	15	2
1	D	81	THR	C-N-CA	6.91	131.45	121.02	15	2
1	D	32	ASN	N-CA-C	6.90	121.86	113.17	3	2
1	B	48	ARG	NE-CZ-NH2	6.90	125.41	119.20	2	2
1	B	34	LEU	N-CA-C	6.90	120.58	112.72	9	1
1	D	47	GLU	CA-C-N	6.89	132.39	120.68	9	4
1	D	47	GLU	C-N-CA	6.89	132.39	120.68	9	4
1	C	46	ASP	CA-C-N	6.88	129.80	120.44	5	2
1	C	46	ASP	C-N-CA	6.88	129.80	120.44	5	2
1	B	28	ASN	CA-C-N	6.88	130.77	120.31	2	1
1	B	28	ASN	C-N-CA	6.88	130.77	120.31	2	1
1	A	78	GLY	CA-C-O	-6.88	114.56	120.89	11	1
1	B	48	ARG	NH1-CZ-NH2	-6.87	110.37	119.30	2	1
1	A	103	VAL	N-CA-CB	6.87	118.41	110.65	14	2
1	C	103	VAL	CB-CA-C	-6.87	103.70	111.80	7	1
1	A	16	HIS	ND1-CG-CD2	6.87	112.97	106.10	15	1
1	A	24	ASP	N-CA-C	6.86	118.84	111.36	7	2
1	D	56	ARG	NE-CZ-NH2	6.86	125.38	119.20	10	1
1	C	15	ARG	NE-CZ-NH2	-6.85	113.03	119.20	15	3
1	C	54	ARG	CA-C-N	6.85	129.85	120.46	13	3
1	C	54	ARG	C-N-CA	6.85	129.85	120.46	13	3
1	D	76	GLY	CA-C-N	6.84	133.72	120.99	10	1
1	D	76	GLY	C-N-CA	6.84	133.72	120.99	10	1
1	C	16	HIS	CB-CG-CD2	-6.84	122.31	131.20	9	7
1	C	97	ARG	CA-C-O	-6.84	112.37	120.10	14	2
1	C	22	PHE	CA-CB-CG	6.83	120.64	113.80	1	2
1	B	104	LEU	CA-C-O	6.83	127.86	120.55	13	1
1	B	40	ASN	CA-C-O	-6.83	113.31	120.55	10	1
1	D	87	ASN	CA-C-O	6.83	127.16	121.02	6	1
1	A	75	LEU	N-CA-C	6.83	121.89	113.50	14	1
1	C	35	HIS	CA-C-N	6.82	129.41	120.26	6	2
1	C	35	HIS	C-N-CA	6.82	129.41	120.26	6	2
1	A	65	GLU	CA-C-N	6.82	131.61	121.72	15	1
1	A	65	GLU	C-N-CA	6.82	131.61	121.72	15	1
1	D	84	ARG	CD-NE-CZ	6.82	133.95	124.40	14	3
1	D	107	SER	CA-C-O	6.82	127.92	119.05	7	1
1	C	2	ALA	N-CA-C	6.82	119.85	110.24	7	2
1	B	100	LEU	CA-C-N	6.81	129.71	120.38	5	2
1	B	100	LEU	C-N-CA	6.81	129.71	120.38	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	16	HIS	CE1-NE2-CD2	-6.81	102.19	109.00	8	1
1	B	36	LEU	O-C-N	6.81	125.76	120.38	7	3
1	B	15	ARG	N-CA-C	6.81	120.46	111.75	9	2
1	C	31	GLN	OE1-CD-NE2	-6.80	115.80	122.60	11	4
1	D	77	ALA	N-CA-CB	-6.80	99.00	110.49	1	1
1	A	77	ALA	CA-C-N	6.80	126.45	119.92	14	2
1	A	77	ALA	C-N-CA	6.80	126.45	119.92	14	2
1	D	36	LEU	CB-CA-C	6.80	123.57	110.17	15	1
1	C	15	ARG	N-CA-CB	6.80	120.22	110.16	12	1
1	B	40	ASN	CA-CB-CG	6.80	119.40	112.60	11	4
1	C	35	HIS	ND1-CG-CD2	6.80	112.90	106.10	3	2
1	C	53	THR	N-CA-C	6.79	119.26	111.11	14	1
1	D	75	LEU	CA-C-O	-6.79	113.28	120.55	13	2
1	C	45	PRO	N-CA-CB	6.78	110.89	103.30	7	3
1	C	37	PRO	N-CA-CB	6.78	110.71	103.39	15	3
1	C	35	HIS	CG-CD2-NE2	-6.77	100.43	107.20	3	2
1	B	81	THR	CA-C-O	-6.77	113.32	120.63	15	2
1	B	74	GLU	N-CA-CB	6.76	119.89	110.90	11	1
1	D	85	GLY	CA-C-O	-6.76	117.18	122.52	13	3
1	C	25	LEU	CA-C-N	6.75	130.57	120.31	7	3
1	C	25	LEU	C-N-CA	6.75	130.57	120.31	7	3
1	D	44	THR	N-CA-C	6.75	119.22	109.84	2	2
1	B	11	MET	CA-C-N	6.75	129.87	120.29	15	2
1	B	11	MET	C-N-CA	6.75	129.87	120.29	15	2
1	C	41	LEU	CA-C-O	6.74	127.94	119.78	3	3
1	C	51	LEU	N-CA-C	6.74	118.42	111.14	13	4
1	A	16	HIS	CA-CB-CG	-6.74	107.06	113.80	14	2
1	D	76	GLY	N-CA-C	6.74	123.95	112.22	2	2
1	B	32	ASN	CA-C-O	-6.74	111.47	119.35	5	1
1	C	65	GLU	CA-C-O	-6.73	111.47	119.15	4	2
1	A	94	VAL	CA-C-N	6.73	129.97	120.28	6	1
1	A	94	VAL	C-N-CA	6.73	129.97	120.28	6	1
1	D	7	TYR	CA-C-O	-6.73	113.45	120.99	8	1
1	B	55	VAL	O-C-N	-6.73	114.90	121.83	15	2
1	A	23	VAL	CA-C-O	-6.72	113.72	120.85	10	1
1	C	95	GLU	CA-C-O	-6.72	112.51	120.10	12	3
1	B	56	ARG	NE-CZ-NH1	6.71	128.21	121.50	2	5
1	B	105	LEU	CA-C-N	6.71	132.76	122.29	14	2
1	B	105	LEU	C-N-CA	6.71	132.76	122.29	14	2
1	D	57	ILE	CA-CB-CG2	6.71	121.91	110.50	10	1
1	C	59	GLU	CB-CG-CD	-6.71	101.19	112.60	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	42	MET	N-CA-C	6.71	121.55	113.23	1	1
1	C	44	THR	CA-C-N	6.71	126.40	119.56	1	2
1	C	44	THR	C-N-CA	6.71	126.40	119.56	1	2
1	B	56	ARG	NE-CZ-NH2	6.70	125.23	119.20	7	3
1	A	62	LEU	CA-C-N	6.70	129.81	120.29	2	2
1	A	62	LEU	C-N-CA	6.70	129.81	120.29	2	2
1	A	14	GLN	CA-C-O	-6.70	113.32	120.42	8	1
1	B	16	HIS	N-CA-C	6.70	119.93	111.69	14	1
1	B	37	PRO	N-CA-CB	6.70	110.45	103.15	9	2
1	C	59	GLU	O-C-N	-6.69	115.17	122.07	12	2
1	B	64	GLY	O-C-N	6.68	129.93	122.31	1	1
1	B	39	LEU	O-C-N	-6.68	114.53	122.15	5	1
1	A	97	ARG	CA-C-N	6.68	129.53	120.38	3	1
1	A	97	ARG	C-N-CA	6.68	129.53	120.38	3	1
1	B	98	GLN	CG-CD-NE2	6.68	126.42	116.40	9	1
1	A	105	LEU	N-CA-C	6.68	122.52	113.97	9	2
1	D	29	ALA	O-C-N	-6.67	115.05	122.12	9	1
1	D	74	GLU	CB-CG-CD	6.67	123.95	112.60	12	1
1	A	106	LYS	N-CA-CB	-6.67	100.25	110.20	15	1
1	B	97	ARG	NE-CZ-NH2	6.67	125.20	119.20	2	8
1	D	99	TRP	CA-C-N	6.67	129.45	120.65	1	1
1	D	99	TRP	C-N-CA	6.67	129.45	120.65	1	1
1	D	59	GLU	O-C-N	-6.67	115.05	122.12	2	1
1	B	16	HIS	CA-C-N	6.67	129.22	120.28	13	1
1	B	16	HIS	C-N-CA	6.67	129.22	120.28	13	1
1	C	99	TRP	CA-C-N	6.67	129.21	120.28	6	1
1	C	99	TRP	C-N-CA	6.67	129.21	120.28	6	1
1	A	86	SER	O-C-N	6.67	129.19	122.12	11	1
1	A	60	GLU	CA-C-O	-6.66	111.05	119.31	1	2
1	A	91	ALA	N-CA-C	6.66	121.42	113.16	12	1
1	A	28	ASN	CA-C-O	6.66	127.47	120.42	12	2
1	B	71	LEU	N-CA-CB	-6.65	99.97	110.22	1	1
1	B	53	THR	CA-C-O	-6.65	113.83	120.82	7	2
1	C	81	THR	OG1-CB-CG2	-6.65	96.00	109.30	11	1
1	D	22	PHE	CA-C-O	-6.64	113.84	120.82	15	3
1	C	48	ARG	CA-C-O	6.64	127.61	120.10	11	2
1	C	77	ALA	N-CA-C	6.64	120.48	112.38	7	1
1	A	41	LEU	N-CA-CB	-6.64	100.31	110.20	5	1
1	A	21	ARG	CA-C-N	6.63	129.17	120.28	9	1
1	A	21	ARG	C-N-CA	6.63	129.17	120.28	9	1
1	B	33	ASP	N-CA-C	6.63	121.14	113.38	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	75	LEU	N-CA-CB	-6.63	100.78	110.53	14	1
1	B	94	VAL	CA-C-N	6.63	129.82	120.28	5	2
1	B	94	VAL	C-N-CA	6.63	129.82	120.28	5	2
1	D	107	SER	N-CA-C	6.62	119.50	111.82	5	2
1	A	83	THR	CA-CB-CG2	6.62	121.76	110.50	11	1
1	D	40	ASN	CA-C-N	6.62	129.39	120.65	13	1
1	D	40	ASN	C-N-CA	6.62	129.39	120.65	13	1
1	A	35	HIS	CA-C-O	-6.62	113.41	120.42	13	2
1	B	24	ASP	CA-CB-CG	-6.62	105.98	112.60	5	2
1	C	67	SER	CA-C-N	6.61	129.44	120.38	8	2
1	C	67	SER	C-N-CA	6.61	129.44	120.38	8	2
1	B	35	HIS	CA-C-N	6.61	127.98	119.78	3	1
1	B	35	HIS	C-N-CA	6.61	127.98	119.78	3	1
1	A	55	VAL	O-C-N	-6.61	115.46	121.87	1	1
1	B	98	GLN	CA-C-N	6.60	131.73	120.71	9	3
1	B	98	GLN	C-N-CA	6.60	131.73	120.71	9	3
1	D	75	LEU	O-C-N	-6.59	113.50	122.33	14	1
1	A	11	MET	O-C-N	-6.58	114.17	122.27	3	1
1	B	65	GLU	O-C-N	-6.58	113.29	122.10	12	1
1	C	80	ALA	CA-C-O	-6.58	113.92	120.82	13	2
1	C	4	GLN	CA-C-N	6.57	132.77	122.26	5	2
1	C	4	GLN	C-N-CA	6.57	132.77	122.26	5	2
1	A	82	ILE	CA-C-O	-6.57	113.89	120.85	11	1
1	B	31	GLN	OE1-CD-NE2	-6.57	116.03	122.60	7	6
1	B	89	LEU	CA-C-O	-6.57	113.59	120.55	3	2
1	A	15	ARG	N-CA-C	-6.56	104.05	111.14	3	2
1	B	13	GLU	CA-C-N	6.56	129.40	120.54	3	2
1	B	13	GLU	C-N-CA	6.56	129.40	120.54	3	2
1	C	100	LEU	O-C-N	-6.56	114.55	122.22	4	3
1	C	81	THR	CA-C-N	6.55	130.92	121.02	15	2
1	C	81	THR	C-N-CA	6.55	130.92	121.02	15	2
1	D	41	LEU	CA-C-N	6.55	131.82	120.68	5	4
1	D	41	LEU	C-N-CA	6.55	131.82	120.68	5	4
1	D	15	ARG	CD-NE-CZ	6.55	133.58	124.40	12	2
1	D	48	ARG	NE-CZ-NH2	-6.55	113.30	119.20	9	2
1	B	29	ALA	CA-C-O	-6.55	113.47	120.42	12	1
1	C	90	LYS	CG-CD-CE	-6.54	96.25	111.30	15	1
1	D	98	GLN	CA-CB-CG	6.54	127.18	114.10	8	1
1	D	29	ALA	CA-C-N	6.54	129.69	120.28	9	1
1	D	29	ALA	C-N-CA	6.54	129.69	120.28	9	1
1	A	102	GLU	N-CA-C	6.53	118.28	111.03	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	63	ARG	CA-C-O	-6.53	112.08	119.79	15	1
1	C	106	LYS	CA-C-O	6.53	128.08	120.96	11	3
1	D	16	HIS	ND1-CE1-NE2	6.53	114.93	108.40	3	1
1	B	32	ASN	O-C-N	-6.53	115.12	122.23	8	1
1	B	85	GLY	CA-C-N	6.52	129.31	120.44	1	2
1	B	85	GLY	C-N-CA	6.52	129.31	120.44	1	2
1	B	21	ARG	NH1-CZ-NH2	-6.52	110.82	119.30	10	6
1	D	13	GLU	CB-CG-CD	6.52	123.69	112.60	14	1
1	B	35	HIS	O-C-N	-6.52	115.21	122.12	3	1
1	D	13	GLU	CB-CA-C	6.52	121.74	110.79	13	1
1	C	32	ASN	OD1-CG-ND2	-6.51	116.09	122.60	15	3
1	B	15	ARG	NE-CZ-NH1	6.51	128.01	121.50	5	3
1	A	71	LEU	CA-C-N	6.51	129.33	120.54	13	2
1	A	71	LEU	C-N-CA	6.51	129.33	120.54	13	2
1	C	49	GLU	CA-C-N	6.51	129.00	120.28	8	4
1	C	49	GLU	C-N-CA	6.51	129.00	120.28	8	4
1	B	50	ALA	CB-CA-C	6.50	121.03	110.95	9	1
1	A	28	ASN	CA-CB-CG	-6.50	106.10	112.60	11	2
1	B	101	GLU	N-CA-C	6.50	119.19	111.33	8	1
1	D	54	ARG	NE-CZ-NH1	6.50	128.00	121.50	6	3
1	D	21	ARG	CA-C-O	-6.49	114.01	120.70	4	2
1	C	91	ALA	CA-C-N	6.49	130.54	120.60	10	2
1	C	91	ALA	C-N-CA	6.49	130.54	120.60	10	2
1	C	53	THR	CA-CB-CG2	6.49	121.54	110.50	6	1
1	D	62	LEU	N-CA-C	-6.49	105.00	113.12	12	2
1	D	97	ARG	CD-NE-CZ	6.49	133.49	124.40	7	2
1	C	53	THR	CA-C-N	6.49	128.97	120.28	1	2
1	C	53	THR	C-N-CA	6.49	128.97	120.28	1	2
1	A	55	VAL	N-CA-C	6.49	117.24	110.62	4	1
1	C	40	ASN	CA-CB-CG	6.49	119.09	112.60	13	2
1	C	47	GLU	CA-C-O	6.49	127.30	120.42	8	2
1	A	99	TRP	CD2-CE3-CZ3	6.48	127.02	118.60	13	2
1	A	100	LEU	N-CA-C	-6.48	104.86	112.89	7	2
1	A	14	GLN	N-CA-C	-6.48	103.45	112.45	3	1
1	A	84	ARG	NE-CZ-NH1	-6.46	115.03	121.50	6	2
1	A	63	ARG	NH1-CZ-NH2	-6.46	110.90	119.30	11	2
1	A	12	ALA	N-CA-C	6.46	120.43	112.54	12	1
1	A	42	MET	CA-C-O	-6.46	111.31	119.31	12	2
1	B	44	THR	N-CA-C	6.45	118.98	110.08	1	1
1	B	84	ARG	NH1-CZ-NH2	-6.45	110.92	119.30	13	2
1	C	48	ARG	O-C-N	6.45	128.95	122.12	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	103	VAL	CA-C-O	-6.45	115.22	120.70	10	1
1	B	11	MET	O-C-N	6.44	130.20	122.27	10	1
1	D	5	SER	CA-C-O	-6.44	114.03	119.76	6	4
1	D	105	LEU	CA-C-N	6.44	132.42	120.95	12	3
1	D	105	LEU	C-N-CA	6.44	132.42	120.95	12	3
1	C	65	GLU	CA-C-N	6.44	129.90	120.82	1	1
1	C	65	GLU	C-N-CA	6.44	129.90	120.82	1	1
1	C	75	LEU	CB-CA-C	6.44	121.01	109.29	5	1
1	B	101	GLU	CA-C-N	6.43	131.62	120.68	3	1
1	B	101	GLU	C-N-CA	6.43	131.62	120.68	3	1
1	D	41	LEU	CA-C-O	-6.43	114.06	120.82	5	1
1	C	2	ALA	N-CA-CB	-6.43	100.64	110.42	8	3
1	A	18	GLU	CA-C-N	6.43	129.18	120.44	5	3
1	A	18	GLU	C-N-CA	6.43	129.18	120.44	5	3
1	D	30	TYR	CA-CB-CG	6.43	125.47	113.90	5	4
1	A	18	GLU	N-CA-C	6.42	118.36	111.36	6	2
1	C	44	THR	CA-C-O	-6.42	114.02	120.64	4	1
1	D	46	ASP	N-CA-C	6.42	120.38	112.54	12	1
1	D	55	VAL	CA-C-O	-6.42	114.73	121.41	4	2
1	B	88	SER	N-CA-C	-6.42	103.79	111.69	7	1
1	D	103	VAL	CA-CB-CG2	6.42	121.32	110.40	9	2
1	D	48	ARG	N-CA-C	6.42	118.36	111.36	15	2
1	A	89	LEU	CA-C-O	-6.42	113.11	120.24	7	1
1	A	99	TRP	CB-CG-CD2	6.42	135.79	126.80	13	1
1	A	85	GLY	CA-C-N	6.42	128.88	120.28	14	3
1	A	85	GLY	C-N-CA	6.42	128.88	120.28	14	3
1	A	102	GLU	CA-C-O	-6.41	112.02	119.78	11	1
1	D	47	GLU	N-CA-C	-6.41	104.38	111.36	6	1
1	D	24	ASP	O-C-N	-6.40	115.17	122.09	14	1
1	C	89	LEU	N-CA-CB	-6.40	100.36	110.28	9	1
1	A	84	ARG	NH1-CZ-NH2	-6.40	110.98	119.30	14	1
1	B	104	LEU	O-C-N	-6.40	114.43	122.17	13	1
1	D	82	ILE	N-CA-C	6.39	120.99	112.04	2	1
1	C	49	GLU	N-CA-C	-6.39	104.31	111.28	3	3
1	A	79	ILE	CA-C-O	-6.39	114.39	121.17	2	1
1	C	30	TYR	O-C-N	-6.39	113.87	122.43	10	1
1	D	81	THR	N-CA-C	6.39	118.32	111.36	5	1
1	C	86	SER	N-CA-C	6.38	119.05	111.71	10	1
1	B	75	LEU	CD1-CG-CD2	-6.38	96.77	110.80	13	1
1	D	14	GLN	O-C-N	-6.37	114.43	122.27	15	2
1	B	96	LEU	N-CA-C	-6.37	104.46	112.93	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	84	ARG	CA-C-N	6.36	127.18	119.99	9	2
1	A	84	ARG	C-N-CA	6.36	127.18	119.99	9	2
1	D	35	HIS	CA-C-O	-6.36	114.14	120.82	10	1
1	B	69	ARG	CA-C-N	6.36	129.09	120.44	4	3
1	B	69	ARG	C-N-CA	6.36	129.09	120.44	4	3
1	D	100	LEU	CA-C-N	6.36	128.80	120.28	3	1
1	D	100	LEU	C-N-CA	6.36	128.80	120.28	3	1
1	B	69	ARG	N-CA-C	6.36	118.21	111.28	5	2
1	B	70	GLU	CA-C-O	-6.35	114.16	120.70	13	1
1	D	39	LEU	CA-C-O	-6.35	113.69	120.42	11	3
1	B	81	THR	CA-CB-OG1	6.34	119.12	109.60	8	1
1	A	37	PRO	CA-C-N	6.34	129.25	120.63	12	2
1	A	37	PRO	C-N-CA	6.34	129.25	120.63	12	2
1	D	42	MET	CA-C-O	-6.34	113.83	120.55	15	2
1	B	87	ASN	OD1-CG-ND2	-6.34	116.26	122.60	10	3
1	C	80	ALA	CA-C-N	6.34	128.77	120.28	5	2
1	C	80	ALA	C-N-CA	6.34	128.77	120.28	5	2
1	C	12	ALA	N-CA-C	6.34	119.00	111.71	8	3
1	D	15	ARG	N-CA-C	6.33	118.99	111.71	1	2
1	B	31	GLN	N-CA-C	6.33	120.47	112.87	10	2
1	A	94	VAL	N-CA-C	6.33	117.84	110.62	10	1
1	A	104	LEU	CB-CA-C	-6.33	98.17	109.24	3	1
1	D	94	VAL	CA-CB-CG2	6.33	121.15	110.40	6	1
1	A	55	VAL	CA-C-N	6.32	129.27	120.29	5	2
1	A	55	VAL	C-N-CA	6.32	129.27	120.29	5	2
1	C	54	ARG	NH1-CZ-NH2	-6.32	111.08	119.30	8	2
1	B	94	VAL	CA-CB-CG2	6.31	121.13	110.40	9	1
1	A	92	ALA	CA-C-O	-6.31	113.49	119.80	13	2
1	A	83	THR	CA-CB-OG1	6.31	119.06	109.60	14	2
1	C	24	ASP	N-CA-C	6.30	118.15	111.28	1	4
1	D	59	GLU	CA-C-N	6.30	128.72	120.28	4	2
1	D	59	GLU	C-N-CA	6.30	128.72	120.28	4	2
1	B	26	LEU	CB-CA-C	6.30	122.23	110.70	5	2
1	B	63	ARG	NE-CZ-NH2	6.30	124.87	119.20	9	2
1	B	34	LEU	CA-C-N	6.29	128.71	120.28	7	3
1	B	34	LEU	C-N-CA	6.29	128.71	120.28	7	3
1	C	5	SER	O-C-N	-6.29	117.45	121.85	9	1
1	B	84	ARG	CB-CG-CD	6.29	125.76	111.30	7	1
1	A	35	HIS	N-CA-CB	6.29	119.09	109.98	3	1
1	D	47	GLU	O-C-N	-6.29	114.98	122.15	6	2
1	A	63	ARG	CA-C-O	-6.28	113.76	120.42	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	61	LEU	N-CA-C	6.28	118.13	111.28	7	1
1	C	82	ILE	N-CA-CB	-6.28	105.31	112.21	6	3
1	B	55	VAL	CA-C-N	6.27	129.31	120.28	4	1
1	B	55	VAL	C-N-CA	6.27	129.31	120.28	4	1
1	B	103	VAL	CA-C-O	-6.27	113.91	121.18	4	1
1	D	76	GLY	O-C-N	6.27	130.16	122.95	5	2
1	A	93	PRO	CA-N-CD	-6.27	103.22	112.00	10	1
1	D	13	GLU	CA-C-N	6.27	128.68	120.28	11	1
1	D	13	GLU	C-N-CA	6.27	128.68	120.28	11	1
1	D	16	HIS	CA-C-O	-6.27	112.39	119.79	3	1
1	D	45	PRO	N-CA-CB	6.27	110.22	103.33	7	1
1	D	97	ARG	NH1-CZ-NH2	-6.26	111.16	119.30	4	2
1	D	30	TYR	CA-C-N	6.26	129.19	120.29	13	2
1	D	30	TYR	C-N-CA	6.26	129.19	120.29	13	2
1	D	96	LEU	CA-C-N	6.26	128.58	120.44	10	1
1	D	96	LEU	C-N-CA	6.26	128.58	120.44	10	1
1	D	89	LEU	CA-C-O	-6.26	113.19	120.20	12	1
1	D	55	VAL	CA-CB-CG1	6.25	121.03	110.40	9	2
1	A	81	THR	CA-CB-OG1	6.25	118.97	109.60	13	1
1	B	20	LEU	CA-C-N	6.25	128.56	120.44	13	1
1	B	20	LEU	C-N-CA	6.25	128.56	120.44	13	1
1	C	41	LEU	CA-C-N	6.24	128.93	120.44	2	1
1	C	41	LEU	C-N-CA	6.24	128.93	120.44	2	1
1	D	82	ILE	CA-C-O	6.24	126.41	119.42	15	1
1	D	95	GLU	N-CA-CB	6.24	119.96	110.42	10	1
1	A	40	ASN	OD1-CG-ND2	-6.23	116.37	122.60	10	2
1	B	44	THR	CA-C-O	-6.23	112.31	121.27	13	3
1	C	48	ARG	CD-NE-CZ	6.22	133.11	124.40	11	1
1	A	98	GLN	CG-CD-NE2	6.22	125.73	116.40	2	2
1	C	19	TRP	N-CA-C	6.22	118.06	111.28	15	3
1	C	69	ARG	NH1-CZ-NH2	-6.21	111.23	119.30	4	2
1	A	37	PRO	N-CA-CB	6.21	110.16	103.33	3	2
1	C	44	THR	CA-CB-OG1	6.20	118.90	109.60	11	1
1	C	28	ASN	CB-CG-ND2	6.20	125.71	116.40	14	1
1	D	32	ASN	CA-C-N	6.20	131.39	122.40	13	1
1	D	32	ASN	C-N-CA	6.20	131.39	122.40	13	1
1	A	79	ILE	CA-C-N	6.20	129.73	120.31	10	1
1	A	79	ILE	C-N-CA	6.20	129.73	120.31	10	1
1	B	58	VAL	O-C-N	-6.20	115.86	121.87	5	1
1	C	87	ASN	CB-CG-ND2	6.20	125.69	116.40	11	1
1	B	23	VAL	CA-CB-CG1	6.20	120.93	110.40	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	101	GLU	N-CA-C	6.19	118.82	111.33	15	2
1	C	106	LYS	CB-CA-C	6.19	118.67	110.06	15	1
1	D	14	GLN	N-CA-C	6.19	118.81	111.33	4	3
1	A	61	LEU	N-CA-C	6.19	118.02	111.28	12	1
1	C	29	ALA	N-CA-C	6.18	118.82	111.71	11	2
1	A	38	LEU	CB-CA-C	6.18	120.53	110.95	12	1
1	B	69	ARG	CA-C-O	6.18	127.06	120.70	6	4
1	B	39	LEU	N-CA-C	6.17	118.09	111.36	9	1
1	A	37	PRO	O-C-N	-6.16	115.15	122.24	13	2
1	A	67	SER	N-CA-C	6.16	119.58	110.46	8	1
1	D	69	ARG	CA-C-O	-6.16	114.31	120.90	10	2
1	B	80	ALA	O-C-N	-6.16	114.22	122.23	3	3
1	D	48	ARG	CD-NE-CZ	6.16	133.03	124.40	10	2
1	C	68	GLN	O-C-N	6.16	128.64	122.12	8	1
1	B	80	ALA	CA-C-O	-6.16	113.89	120.42	12	1
1	A	83	THR	OG1-CB-CG2	-6.15	97.00	109.30	14	1
1	D	57	ILE	O-C-N	6.15	128.16	121.83	1	1
1	D	77	ALA	CA-C-N	6.15	131.32	120.74	5	1
1	D	77	ALA	C-N-CA	6.15	131.32	120.74	5	1
1	D	60	GLU	O-C-N	-6.15	115.03	122.22	3	1
1	B	17	GLN	N-CA-C	6.15	118.06	111.36	9	1
1	C	92	ALA	O-C-N	-6.15	114.65	121.66	15	2
1	B	56	ARG	CA-C-N	6.15	128.38	120.70	14	2
1	B	56	ARG	C-N-CA	6.15	128.38	120.70	14	2
1	B	25	LEU	CA-C-N	6.15	128.76	120.65	6	2
1	B	25	LEU	C-N-CA	6.15	128.76	120.65	6	2
1	A	63	ARG	CD-NE-CZ	6.14	133.00	124.40	1	2
1	C	35	HIS	O-C-N	-6.14	115.61	122.12	10	2
1	C	57	ILE	CA-C-N	6.13	128.51	120.60	6	2
1	C	57	ILE	C-N-CA	6.13	128.51	120.60	6	2
1	A	94	VAL	CA-C-O	-6.13	114.57	120.95	8	3
1	C	84	ARG	NE-CZ-NH2	6.13	124.72	119.20	10	3
1	A	89	LEU	N-CA-C	6.12	119.22	111.69	5	2
1	A	75	LEU	O-C-N	-6.12	114.82	122.35	7	1
1	C	2	ALA	CB-CA-C	6.12	119.88	109.72	5	2
1	D	74	GLU	CB-CA-C	6.12	119.93	109.65	13	1
1	B	11	MET	N-CA-C	-6.12	103.95	112.45	3	1
1	B	47	GLU	CA-C-O	6.12	126.90	120.42	7	2
1	C	97	ARG	CA-C-N	6.11	128.79	120.54	10	3
1	C	97	ARG	C-N-CA	6.11	128.79	120.54	10	3
1	A	35	HIS	CA-CB-CG	6.11	119.91	113.80	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	55	VAL	N-CA-C	6.11	116.28	110.42	3	4
1	A	77	ALA	N-CA-C	6.11	117.98	109.31	15	3
1	C	30	TYR	N-CA-C	-6.11	104.53	111.07	12	2
1	A	24	ASP	O-C-N	-6.11	114.24	122.43	13	1
1	C	97	ARG	CD-NE-CZ	6.11	132.95	124.40	4	2
1	B	57	ILE	CA-C-O	-6.11	114.38	120.85	6	1
1	A	19	TRP	CD2-CE3-CZ3	6.11	126.54	118.60	13	1
1	C	9	ALA	CA-C-O	-6.11	112.95	119.97	13	1
1	A	11	MET	CA-C-O	-6.10	113.95	120.42	7	1
1	B	73	ASN	CB-CG-ND2	6.10	125.56	116.40	2	1
1	A	62	LEU	CA-C-O	-6.10	114.42	120.70	13	2
1	B	63	ARG	CD-NE-CZ	6.09	132.93	124.40	9	2
1	A	72	LYS	CA-C-O	-6.09	113.48	120.24	15	1
1	D	84	ARG	N-CA-CB	6.09	118.72	110.38	2	2
1	B	26	LEU	O-C-N	6.08	128.34	122.07	9	1
1	B	93	PRO	O-C-N	-6.08	115.59	123.00	8	2
1	D	78	GLY	CA-C-O	-6.07	112.48	119.65	13	2
1	B	50	ALA	CA-C-O	-6.07	114.62	121.00	11	3
1	B	35	HIS	ND1-CE1-NE2	6.07	114.47	108.40	2	2
1	C	96	LEU	CA-C-N	6.07	129.24	120.38	3	4
1	C	96	LEU	C-N-CA	6.07	129.24	120.38	3	4
1	B	92	ALA	N-CA-C	6.07	117.54	109.83	14	1
1	B	18	GLU	O-C-N	-6.07	114.81	122.27	2	1
1	A	34	LEU	CA-C-N	6.07	128.90	120.29	15	2
1	A	34	LEU	C-N-CA	6.07	128.90	120.29	15	2
1	C	21	ARG	N-CA-C	6.06	118.85	111.82	9	2
1	B	36	LEU	N-CA-CB	6.06	116.15	110.39	5	1
1	A	58	VAL	CA-CB-CG1	6.06	120.70	110.40	15	1
1	A	64	GLY	N-CA-C	6.06	123.72	115.30	7	2
1	B	88	SER	CA-C-O	6.06	126.93	119.97	8	2
1	B	18	GLU	N-CA-C	6.05	117.88	111.28	14	2
1	C	25	LEU	CD1-CG-CD2	-6.05	97.49	110.80	3	1
1	B	84	ARG	CA-CB-CG	-6.04	102.01	114.10	5	1
1	C	15	ARG	NH1-CZ-NH2	-6.04	111.44	119.30	9	3
1	D	35	HIS	CE1-NE2-CD2	-6.04	102.96	109.00	1	1
1	A	106	LYS	CB-CA-C	6.04	119.21	109.07	1	1
1	C	22	PHE	N-CA-C	6.03	118.63	111.33	8	2
1	C	22	PHE	CA-C-N	6.03	128.28	120.56	14	2
1	C	22	PHE	C-N-CA	6.03	128.28	120.56	14	2
1	C	75	LEU	N-CA-C	6.03	120.77	113.41	13	2
1	D	101	GLU	CB-CG-CD	-6.03	102.35	112.60	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	16	HIS	CG-CD2-NE2	-6.03	101.17	107.20	10	1
1	D	31	GLN	CA-C-O	-6.02	112.31	119.35	10	1
1	D	83	THR	O-C-N	-6.02	114.62	122.20	15	1
1	D	54	ARG	CA-C-N	6.01	128.14	120.56	1	1
1	D	54	ARG	C-N-CA	6.01	128.14	120.56	1	1
1	C	30	TYR	CA-C-O	6.01	126.77	119.49	14	2
1	D	88	SER	O-C-N	-6.01	115.59	122.68	5	1
1	A	14	GLN	O-C-N	-6.01	115.75	122.12	13	1
1	A	82	ILE	CB-CA-C	6.01	119.89	112.02	3	2
1	B	105	LEU	CA-C-O	6.01	126.89	120.10	2	1
1	D	36	LEU	O-C-N	-6.01	114.41	121.32	11	1
1	B	26	LEU	CD1-CG-CD2	-6.00	97.59	110.80	3	1
1	C	82	ILE	N-CA-C	6.00	116.78	110.72	4	1
1	B	61	LEU	CB-CA-C	6.00	121.05	110.37	9	1
1	C	74	GLU	CA-C-O	-6.00	111.93	120.51	14	1
1	A	20	LEU	N-CA-C	6.00	119.70	112.38	3	1
1	C	32	ASN	CA-C-N	6.00	131.10	122.40	5	1
1	C	32	ASN	C-N-CA	6.00	131.10	122.40	5	1
1	A	66	MET	CB-CA-C	6.00	119.42	109.53	6	1
1	B	86	SER	N-CA-C	5.99	117.81	111.28	7	1
1	A	65	GLU	N-CA-C	5.98	120.44	113.20	13	1
1	C	7	TYR	CA-C-N	5.98	131.31	121.86	14	1
1	C	7	TYR	C-N-CA	5.98	131.31	121.86	14	1
1	A	52	GLY	CA-C-N	5.98	128.89	120.28	2	1
1	A	52	GLY	C-N-CA	5.98	128.89	120.28	2	1
1	C	57	ILE	CA-C-O	-5.98	114.42	121.05	10	1
1	B	77	ALA	CA-C-O	5.97	126.85	120.46	6	1
1	C	23	VAL	CA-CB-CG1	5.97	120.56	110.40	11	2
1	B	103	VAL	CA-CB-CG2	-5.97	100.25	110.40	15	1
1	B	17	GLN	O-C-N	-5.97	115.79	122.12	4	2
1	A	35	HIS	CA-C-N	5.97	127.18	119.78	8	1
1	A	35	HIS	C-N-CA	5.97	127.18	119.78	8	1
1	C	20	LEU	CA-C-O	-5.97	113.36	120.10	4	1
1	A	60	GLU	CA-C-N	5.97	128.55	120.44	15	1
1	A	60	GLU	C-N-CA	5.97	128.55	120.44	15	1
1	B	96	LEU	CA-C-O	-5.96	114.54	120.80	1	1
1	C	87	ASN	CA-C-N	5.96	130.95	120.87	8	1
1	C	87	ASN	C-N-CA	5.96	130.95	120.87	8	1
1	C	46	ASP	CA-C-O	-5.96	114.23	120.55	11	1
1	B	73	ASN	CA-C-O	5.96	125.69	119.14	3	1
1	A	35	HIS	O-C-N	-5.95	115.94	122.07	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	48	ARG	NE-CZ-NH2	5.95	124.56	119.20	12	2
1	B	69	ARG	CD-NE-CZ	5.95	132.74	124.40	11	1
1	B	29	ALA	CA-C-N	5.95	128.18	120.44	15	2
1	B	29	ALA	C-N-CA	5.95	128.18	120.44	15	2
1	A	51	LEU	CA-C-O	-5.95	113.53	120.20	11	1
1	D	60	GLU	N-CA-C	5.95	119.01	111.69	13	2
1	A	17	GLN	CA-C-N	5.95	128.73	120.29	14	2
1	A	17	GLN	C-N-CA	5.95	128.73	120.29	14	2
1	C	83	THR	CA-C-N	5.94	131.86	122.94	14	1
1	C	83	THR	C-N-CA	5.94	131.86	122.94	14	1
1	D	12	ALA	CB-CA-C	5.94	120.65	110.79	5	1
1	B	16	HIS	CA-CB-CG	-5.94	107.86	113.80	10	1
1	D	99	TRP	CH2-CZ2-CE2	5.94	125.22	117.50	11	1
1	C	48	ARG	NE-CZ-NH2	-5.94	113.86	119.20	2	3
1	A	56	ARG	CA-CB-CG	-5.93	102.23	114.10	6	1
1	A	71	LEU	CB-CA-C	5.93	120.64	110.79	8	1
1	C	17	GLN	CA-C-N	5.93	128.23	120.28	10	2
1	C	17	GLN	C-N-CA	5.93	128.23	120.28	10	2
1	D	15	ARG	NE-CZ-NH1	5.93	127.43	121.50	5	3
1	B	12	ALA	N-CA-C	5.92	118.22	111.11	8	1
1	B	10	ALA	N-CA-C	5.92	118.49	111.33	1	2
1	C	92	ALA	CA-C-N	5.92	126.22	119.83	15	2
1	C	92	ALA	C-N-CA	5.92	126.22	119.83	15	2
1	B	60	GLU	CA-C-O	-5.91	113.17	119.97	10	1
1	A	91	ALA	N-CA-CB	-5.91	101.39	110.44	15	1
1	C	91	ALA	N-CA-C	5.91	121.53	113.97	5	1
1	D	70	GLU	N-CA-C	5.91	118.96	111.69	3	2
1	B	91	ALA	CB-CA-C	5.91	121.33	110.11	2	1
1	C	4	GLN	CB-CG-CD	-5.91	102.56	112.60	14	1
1	D	20	LEU	CA-C-N	5.90	130.58	120.72	8	1
1	D	20	LEU	C-N-CA	5.90	130.58	120.72	8	1
1	D	23	VAL	CA-C-N	5.90	128.19	120.28	13	2
1	D	23	VAL	C-N-CA	5.90	128.19	120.28	13	2
1	B	54	ARG	O-C-N	-5.90	115.01	122.27	14	1
1	A	27	LYS	CA-C-O	5.90	127.00	120.63	10	1
1	D	35	HIS	N-CA-C	5.89	118.21	111.02	1	1
1	C	16	HIS	CG-CD2-NE2	-5.89	101.31	107.20	15	2
1	C	103	VAL	N-CA-CB	-5.89	105.74	111.57	10	1
1	D	103	VAL	CB-CA-C	5.89	116.25	111.06	11	1
1	B	81	THR	N-CA-C	5.89	118.18	111.11	4	1
1	A	90	LYS	CA-C-O	-5.89	112.14	119.38	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	103	VAL	CG1-CB-CG2	-5.89	97.85	110.80	12	1
1	B	55	VAL	N-CA-CB	5.89	117.04	110.51	6	2
1	B	58	VAL	CA-C-N	5.89	128.97	120.79	2	1
1	B	58	VAL	C-N-CA	5.89	128.97	120.79	2	1
1	D	93	PRO	N-CD-CG	5.88	110.86	103.80	5	2
1	B	100	LEU	O-C-N	-5.88	115.44	122.15	15	1
1	C	25	LEU	N-CA-C	-5.88	104.50	111.03	9	1
1	A	48	ARG	CA-C-O	-5.88	114.64	120.70	5	2
1	A	52	GLY	N-CA-C	5.88	120.00	112.83	4	2
1	C	16	HIS	N-CA-C	5.88	118.44	111.33	7	2
1	A	55	VAL	CA-C-O	-5.88	115.16	121.27	2	3
1	A	21	ARG	N-CA-C	5.88	118.44	111.33	9	2
1	A	100	LEU	CA-C-N	5.88	128.74	120.28	7	1
1	A	100	LEU	C-N-CA	5.88	128.74	120.28	7	1
1	D	81	THR	CA-CB-CG2	5.87	120.48	110.50	12	3
1	A	70	GLU	N-CA-C	-5.87	105.78	113.12	9	1
1	C	1	MET	CA-C-N	5.87	129.05	120.71	5	1
1	C	1	MET	C-N-CA	5.87	129.05	120.71	5	1
1	A	79	ILE	O-C-N	-5.87	115.94	121.87	7	1
1	C	28	ASN	CA-C-N	5.86	128.72	120.28	8	2
1	C	28	ASN	C-N-CA	5.86	128.72	120.28	8	2
1	B	103	VAL	CB-CA-C	-5.86	104.39	112.24	12	1
1	C	77	ALA	CA-C-O	5.85	126.56	119.31	9	1
1	B	10	ALA	O-C-N	-5.85	116.05	122.07	2	2
1	D	57	ILE	CA-C-N	5.85	127.93	120.56	14	2
1	D	57	ILE	C-N-CA	5.85	127.93	120.56	14	2
1	D	88	SER	N-CA-C	5.84	118.42	110.35	1	3
1	D	23	VAL	CA-C-O	-5.84	114.87	120.95	14	2
1	A	82	ILE	N-CA-C	-5.84	105.15	110.82	15	1
1	B	57	ILE	N-CA-C	-5.84	104.82	110.72	6	1
1	C	21	ARG	CA-C-N	5.84	128.11	120.28	6	1
1	C	21	ARG	C-N-CA	5.84	128.11	120.28	6	1
1	B	37	PRO	N-CA-C	5.84	121.54	113.65	15	1
1	D	93	PRO	N-CA-CB	5.84	109.38	103.25	13	2
1	A	47	GLU	N-CA-CB	5.84	118.64	109.94	7	1
1	B	36	LEU	CA-C-N	5.83	125.70	119.28	5	3
1	B	36	LEU	C-N-CA	5.83	125.70	119.28	5	3
1	C	71	LEU	O-C-N	-5.83	115.09	122.27	5	1
1	B	35	HIS	ND1-CG-CD2	5.83	111.93	106.10	11	5
1	B	15	ARG	N-CA-CB	5.83	118.79	110.16	3	1
1	D	8	SER	N-CA-C	5.83	118.68	110.23	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	16	HIS	ND1-CE1-NE2	5.83	114.23	108.40	5	1
1	C	91	ALA	N-CA-CB	-5.83	100.64	110.49	6	1
1	A	88	SER	N-CA-C	5.83	117.71	111.36	11	2
1	B	63	ARG	N-CA-C	5.83	118.86	111.69	10	2
1	A	16	HIS	CB-CG-ND1	5.82	131.43	122.70	2	1
1	A	82	ILE	CA-CB-CG1	5.82	120.30	110.40	9	2
1	A	103	VAL	CA-C-O	-5.82	113.46	121.15	12	1
1	B	52	GLY	N-CA-C	5.82	119.72	112.73	6	1
1	C	45	PRO	CA-C-N	5.82	128.55	120.29	9	2
1	C	45	PRO	C-N-CA	5.82	128.55	120.29	9	2
1	A	47	GLU	O-C-N	-5.82	114.67	122.23	10	1
1	D	106	LYS	N-CA-C	5.82	117.83	110.33	11	1
1	C	25	LEU	O-C-N	-5.82	115.95	122.12	14	2
1	A	86	SER	CA-C-O	-5.82	113.53	120.10	10	2
1	A	40	ASN	N-CA-C	5.81	119.47	112.38	1	1
1	D	97	ARG	CB-CA-C	5.81	120.43	110.79	1	1
1	A	15	ARG	CD-NE-CZ	5.81	132.53	124.40	12	1
1	B	35	HIS	CE1-NE2-CD2	-5.81	103.19	109.00	2	1
1	D	53	THR	CA-C-N	5.81	128.64	120.28	8	1
1	D	53	THR	C-N-CA	5.81	128.64	120.28	8	1
1	B	72	LYS	O-C-N	5.81	128.13	122.09	10	1
1	C	87	ASN	N-CA-C	5.81	120.52	113.38	11	1
1	D	64	GLY	O-C-N	-5.81	117.81	122.51	12	1
1	D	87	ASN	N-CA-CB	-5.80	103.53	111.65	10	2
1	D	34	LEU	CD1-CG-CD2	-5.80	98.03	110.80	10	1
1	C	16	HIS	CB-CG-ND1	5.80	131.41	122.70	9	1
1	A	99	TRP	CA-C-O	5.80	127.56	120.31	10	1
1	A	25	LEU	CD1-CG-CD2	-5.80	98.03	110.80	15	1
1	C	69	ARG	CA-C-N	5.80	128.52	120.29	11	2
1	C	69	ARG	C-N-CA	5.80	128.52	120.29	11	2
1	A	60	GLU	N-CA-C	5.80	118.38	111.71	3	1
1	D	18	GLU	CA-C-O	5.80	126.64	119.97	12	1
1	A	18	GLU	N-CA-CB	-5.79	101.61	110.01	10	1
1	D	44	THR	CA-C-O	-5.79	114.15	120.87	3	3
1	A	57	ILE	CB-CA-C	5.79	119.96	112.14	9	3
1	B	52	GLY	CA-C-O	-5.79	114.75	121.00	9	2
1	B	54	ARG	N-CA-C	5.79	118.37	111.71	1	1
1	A	104	LEU	N-CA-C	5.79	118.81	111.69	9	1
1	D	95	GLU	CA-CB-CG	5.79	125.67	114.10	5	2
1	D	58	VAL	CA-C-N	5.79	127.96	120.44	9	1
1	D	58	VAL	C-N-CA	5.79	127.96	120.44	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	71	LEU	CA-C-N	5.78	128.34	120.54	10	3
1	B	71	LEU	C-N-CA	5.78	128.34	120.54	10	3
1	C	44	THR	N-CA-C	5.78	117.87	109.84	2	1
1	A	103	VAL	O-C-N	-5.78	115.35	122.57	5	2
1	D	99	TRP	CZ3-CH2-CZ2	-5.77	114.00	121.50	12	1
1	A	35	HIS	N-CA-C	5.77	117.37	111.14	14	1
1	C	46	ASP	N-CA-C	5.77	117.57	111.28	8	1
1	A	69	ARG	N-CA-C	5.77	119.79	112.87	3	2
1	D	96	LEU	N-CA-CB	-5.77	101.65	110.01	2	1
1	B	44	THR	CA-C-N	5.76	127.05	119.84	7	3
1	B	44	THR	C-N-CA	5.76	127.05	119.84	7	3
1	A	71	LEU	N-CA-C	5.76	119.13	111.75	5	1
1	D	35	HIS	CB-CG-ND1	5.76	131.34	122.70	14	3
1	D	96	LEU	O-C-N	-5.76	116.14	122.07	4	1
1	C	90	LYS	N-CA-C	5.76	120.01	112.92	8	2
1	C	95	GLU	CB-CG-CD	5.76	122.39	112.60	2	1
1	A	41	LEU	CA-C-N	5.76	129.07	120.31	11	1
1	A	41	LEU	C-N-CA	5.76	129.07	120.31	11	1
1	D	74	GLU	CA-C-N	5.76	128.47	120.29	12	1
1	D	74	GLU	C-N-CA	5.76	128.47	120.29	12	1
1	D	79	ILE	O-C-N	-5.76	116.08	121.90	15	1
1	B	67	SER	N-CA-C	5.75	118.12	110.53	7	2
1	B	39	LEU	CA-C-N	5.75	130.46	120.68	6	3
1	B	39	LEU	C-N-CA	5.75	130.46	120.68	6	3
1	D	23	VAL	O-C-N	-5.75	115.30	121.80	4	1
1	D	6	PRO	N-CA-C	5.75	121.10	113.57	9	1
1	B	51	LEU	CB-CA-C	5.75	119.90	110.88	15	1
1	A	19	TRP	CB-CG-CD2	5.75	134.85	126.80	3	1
1	A	16	HIS	CG-CD2-NE2	-5.75	101.45	107.20	15	1
1	C	63	ARG	CD-NE-CZ	5.75	132.44	124.40	2	2
1	C	27	LYS	N-CA-C	5.74	117.62	111.36	1	1
1	A	73	ASN	CA-C-N	5.74	128.55	120.28	10	1
1	A	73	ASN	C-N-CA	5.74	128.55	120.28	10	1
1	C	42	MET	CA-C-O	-5.74	112.19	119.31	4	1
1	A	76	GLY	CA-C-N	5.74	130.40	122.77	7	1
1	A	76	GLY	C-N-CA	5.74	130.40	122.77	7	1
1	A	15	ARG	CA-CB-CG	5.74	125.58	114.10	12	1
1	C	79	ILE	N-CA-C	5.74	117.16	110.62	3	1
1	D	62	LEU	CA-C-N	5.74	128.44	120.29	6	1
1	D	62	LEU	C-N-CA	5.74	128.44	120.29	6	1
1	C	53	THR	CA-C-O	-5.74	114.34	120.42	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	57	ILE	N-CA-CB	5.73	117.26	110.55	13	1
1	B	46	ASP	CA-C-O	5.73	126.63	120.55	15	1
1	B	19	TRP	NE1-CE2-CZ2	5.73	138.69	130.10	8	1
1	B	64	GLY	CA-C-O	-5.73	112.91	118.98	9	1
1	A	12	ALA	CA-C-N	5.73	128.23	120.38	8	1
1	A	12	ALA	C-N-CA	5.73	128.23	120.38	8	1
1	C	22	PHE	CA-C-O	-5.72	114.48	120.55	4	1
1	D	48	ARG	O-C-N	5.72	128.67	122.15	15	2
1	D	40	ASN	CB-CA-C	5.72	121.65	110.67	3	1
1	B	22	PHE	O-C-N	5.72	127.96	122.07	9	2
1	B	63	ARG	O-C-N	5.72	130.02	122.30	15	1
1	B	95	GLU	CA-C-N	5.71	128.21	120.44	9	1
1	B	95	GLU	C-N-CA	5.71	128.21	120.44	9	1
1	D	94	VAL	CG1-CB-CG2	-5.71	98.23	110.80	12	1
1	C	8	SER	O-C-N	-5.71	116.39	123.36	9	1
1	B	99	TRP	CD2-CE2-CZ2	-5.71	116.69	122.40	15	1
1	B	45	PRO	N-CA-CB	5.71	109.38	103.15	15	3
1	C	40	ASN	CA-C-N	5.71	128.21	120.44	1	1
1	C	40	ASN	C-N-CA	5.71	128.21	120.44	1	1
1	C	76	GLY	O-C-N	-5.71	116.49	122.60	11	1
1	C	98	GLN	O-C-N	5.71	128.19	122.03	6	3
1	A	25	LEU	CA-C-N	5.71	127.93	120.28	10	1
1	A	25	LEU	C-N-CA	5.71	127.93	120.28	10	1
1	B	50	ALA	O-C-N	5.71	127.97	122.03	11	1
1	D	44	THR	CA-CB-CG2	5.70	120.19	110.50	7	2
1	A	42	MET	N-CA-C	5.70	118.43	111.82	7	2
1	A	70	GLU	CA-C-O	-5.70	113.91	120.24	10	1
1	D	87	ASN	CA-CB-CG	5.70	118.30	112.60	10	1
1	A	99	TRP	CA-C-N	5.69	128.37	120.29	1	1
1	A	99	TRP	C-N-CA	5.69	128.37	120.29	1	1
1	C	20	LEU	CA-C-N	5.69	128.17	120.38	3	1
1	C	20	LEU	C-N-CA	5.69	128.17	120.38	3	1
1	B	19	TRP	O-C-N	-5.69	116.17	122.09	4	2
1	D	53	THR	CA-CB-CG2	5.69	120.17	110.50	9	1
1	A	29	ALA	N-CA-C	5.68	117.48	111.28	12	1
1	C	19	TRP	CA-C-O	-5.68	114.52	120.55	15	1
1	B	25	LEU	N-CA-C	-5.68	104.99	111.07	12	1
1	D	51	LEU	CA-C-N	5.68	126.28	119.98	7	2
1	D	51	LEU	C-N-CA	5.68	126.28	119.98	7	2
1	D	43	LEU	CA-C-O	-5.68	114.69	120.71	10	1
1	C	99	TRP	N-CA-C	5.68	117.47	111.28	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	60	GLU	CA-C-O	-5.68	114.40	120.42	10	3
1	B	66	MET	CA-CB-CG	5.67	125.44	114.10	15	2
1	C	60	GLU	CA-C-N	5.66	128.33	120.29	7	1
1	C	60	GLU	C-N-CA	5.66	128.33	120.29	7	1
1	D	34	LEU	N-CA-C	5.66	119.17	112.72	6	1
1	C	21	ARG	NH1-CZ-NH2	-5.66	111.94	119.30	2	1
1	A	38	LEU	CA-C-O	-5.66	114.42	120.42	9	2
1	B	83	THR	O-C-N	-5.66	116.24	122.07	3	1
1	B	92	ALA	CB-CA-C	5.66	118.58	109.41	3	1
1	D	95	GLU	N-CA-C	-5.66	106.92	113.88	4	1
1	B	31	GLN	CA-C-N	5.66	131.26	122.49	6	1
1	B	31	GLN	C-N-CA	5.66	131.26	122.49	6	1
1	C	50	ALA	O-C-N	-5.66	116.15	122.03	10	1
1	D	51	LEU	N-CA-C	5.66	118.21	111.71	8	1
1	B	13	GLU	CA-C-O	5.66	126.47	119.97	10	1
1	C	54	ARG	NE-CZ-NH1	5.66	127.16	121.50	15	2
1	B	107	SER	O-C-N	-5.65	115.56	122.34	9	1
1	C	11	MET	O-C-N	-5.65	115.61	122.22	4	1
1	C	19	TRP	CA-CB-CG	5.65	124.33	113.60	9	1
1	D	10	ALA	CA-C-N	5.65	130.24	120.58	9	2
1	D	10	ALA	C-N-CA	5.65	130.24	120.58	9	2
1	B	18	GLU	N-CA-CB	-5.64	101.79	110.20	7	1
1	D	66	MET	N-CA-C	5.64	118.11	110.88	12	1
1	D	91	ALA	CA-C-O	-5.64	112.41	118.79	15	2
1	B	21	ARG	O-C-N	-5.64	116.00	122.09	10	1
1	B	38	LEU	O-C-N	-5.64	115.72	122.15	15	1
1	D	16	HIS	CA-C-N	5.64	128.88	120.31	5	1
1	D	16	HIS	C-N-CA	5.64	128.88	120.31	5	1
1	A	67	SER	CA-C-N	5.64	128.11	120.38	5	1
1	A	67	SER	C-N-CA	5.64	128.11	120.38	5	1
1	B	37	PRO	N-CD-CG	5.63	111.65	103.20	2	3
1	A	98	GLN	O-C-N	-5.63	114.89	122.43	8	1
1	D	102	GLU	CA-C-N	5.63	128.12	122.66	13	1
1	D	102	GLU	C-N-CA	5.63	128.12	122.66	13	1
1	C	51	LEU	CA-C-N	5.63	126.19	119.94	11	1
1	C	51	LEU	C-N-CA	5.63	126.19	119.94	11	1
1	B	53	THR	O-C-N	-5.63	114.89	122.43	8	1
1	C	35	HIS	CA-C-O	5.62	126.73	120.82	8	1
1	B	99	TRP	CE2-CD2-CE3	-5.62	113.18	118.80	6	1
1	D	36	LEU	CA-C-N	5.62	125.47	119.28	10	1
1	D	36	LEU	C-N-CA	5.62	125.47	119.28	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	30	TYR	CA-C-N	5.62	129.60	120.60	13	2
1	C	30	TYR	C-N-CA	5.62	129.60	120.60	13	2
1	D	97	ARG	CA-C-N	5.62	128.37	120.28	6	2
1	D	97	ARG	C-N-CA	5.62	128.37	120.28	6	2
1	A	98	GLN	CA-C-O	5.62	126.29	119.38	8	1
1	D	83	THR	CA-CB-OG1	5.62	118.02	109.60	7	1
1	C	36	LEU	O-C-N	-5.61	115.95	120.38	15	1
1	B	48	ARG	CA-C-N	5.61	127.80	120.28	7	1
1	B	48	ARG	C-N-CA	5.61	127.80	120.28	7	1
1	A	35	HIS	ND1-CG-CD2	5.61	111.71	106.10	13	1
1	C	84	ARG	CA-C-O	-5.61	114.82	121.66	4	1
1	D	17	GLN	CA-C-N	5.61	128.83	120.31	5	1
1	D	17	GLN	C-N-CA	5.61	128.83	120.31	5	1
1	D	58	VAL	N-CA-C	5.61	118.10	111.09	3	1
1	C	12	ALA	O-C-N	-5.61	115.38	122.27	6	1
1	D	77	ALA	N-CA-C	5.61	119.60	112.87	10	1
1	D	101	GLU	N-CA-C	5.60	118.15	111.71	8	3
1	D	26	LEU	N-CA-C	5.60	117.06	111.07	8	1
1	B	22	PHE	CA-C-O	-5.60	114.94	120.82	9	1
1	A	50	ALA	CA-C-O	-5.60	114.93	120.70	11	1
1	B	22	PHE	CA-CB-CG	5.60	119.40	113.80	9	2
1	A	84	ARG	CA-C-O	-5.59	113.78	120.10	11	2
1	A	48	ARG	NH1-CZ-NH2	-5.59	112.03	119.30	10	2
1	D	50	ALA	O-C-N	-5.59	115.39	122.27	12	1
1	A	90	LYS	CA-CB-CG	-5.59	102.92	114.10	11	1
1	B	37	PRO	O-C-N	-5.59	115.01	122.22	6	1
1	B	13	GLU	CB-CA-C	5.59	120.07	110.79	14	1
1	C	69	ARG	CD-NE-CZ	5.59	132.23	124.40	14	1
1	B	10	ALA	CA-C-N	5.59	128.80	120.31	2	1
1	B	10	ALA	C-N-CA	5.59	128.80	120.31	2	1
1	A	61	LEU	CA-C-N	5.58	128.22	120.29	15	1
1	A	61	LEU	C-N-CA	5.58	128.22	120.29	15	1
1	A	81	THR	N-CA-C	5.58	117.36	111.28	4	1
1	B	26	LEU	CA-C-O	-5.58	114.50	120.42	11	2
1	C	74	GLU	CA-C-N	5.58	128.03	120.44	6	1
1	C	74	GLU	C-N-CA	5.58	128.03	120.44	6	1
1	A	17	GLN	N-CA-C	-5.58	105.28	111.36	13	1
1	A	27	LYS	O-C-N	-5.58	116.21	122.12	10	1
1	D	91	ALA	N-CA-CB	-5.58	102.49	110.80	7	1
1	C	47	GLU	CA-C-N	5.58	127.69	120.44	9	1
1	C	47	GLU	C-N-CA	5.58	127.69	120.44	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	72	LYS	CB-CA-C	5.58	119.71	110.90	12	1
1	A	30	TYR	N-CA-C	5.57	118.07	111.33	15	2
1	C	17	GLN	CA-C-O	-5.57	112.75	119.49	10	2
1	D	98	GLN	CG-CD-NE2	5.57	124.75	116.40	6	1
1	D	27	LYS	N-CA-CB	-5.56	101.92	110.16	10	1
1	C	26	LEU	CB-CA-C	5.56	121.34	110.67	7	1
1	D	79	ILE	CA-C-N	5.56	130.08	120.58	7	3
1	D	79	ILE	C-N-CA	5.56	130.08	120.58	7	3
1	B	46	ASP	N-CA-C	5.56	117.34	111.28	15	1
1	B	34	LEU	CB-CA-C	5.55	119.95	110.56	8	1
1	B	51	LEU	CA-C-O	-5.55	114.63	120.63	8	1
1	B	84	ARG	CA-C-O	-5.55	114.63	120.63	15	2
1	C	97	ARG	O-C-N	5.55	127.79	122.07	13	1
1	D	13	GLU	N-CA-CB	-5.55	101.11	110.49	3	1
1	D	94	VAL	CA-C-N	5.55	130.07	120.58	5	1
1	D	94	VAL	C-N-CA	5.55	130.07	120.58	5	1
1	D	36	LEU	CA-C-O	-5.55	113.53	118.63	14	1
1	A	19	TRP	N-CA-C	5.54	117.01	110.97	10	2
1	B	59	GLU	O-C-N	-5.54	116.36	122.07	15	2
1	D	54	ARG	CD-NE-CZ	5.54	132.16	124.40	12	2
1	B	81	THR	OG1-CB-CG2	-5.54	98.23	109.30	12	1
1	B	52	GLY	CA-C-N	5.54	127.64	120.44	14	1
1	B	52	GLY	C-N-CA	5.54	127.64	120.44	14	1
1	B	32	ASN	CB-CA-C	5.53	119.73	110.44	10	1
1	A	58	VAL	O-C-N	5.53	127.45	121.87	4	2
1	B	57	ILE	CA-CB-CG2	5.53	119.90	110.50	13	1
1	B	108	ASP	CB-CA-C	5.53	120.60	110.10	1	1
1	C	6	PRO	N-CA-CB	5.52	109.56	103.26	15	1
1	D	28	ASN	OD1-CG-ND2	-5.52	117.08	122.60	14	2
1	B	99	TRP	NE1-CE2-CZ2	5.52	138.38	130.10	13	3
1	C	75	LEU	CA-C-N	5.52	130.83	120.07	15	2
1	C	75	LEU	C-N-CA	5.52	130.83	120.07	15	2
1	A	38	LEU	N-CA-C	5.52	117.38	111.36	10	2
1	B	35	HIS	CA-CB-CG	5.52	119.32	113.80	3	1
1	C	99	TRP	NE1-CE2-CD2	-5.52	100.23	107.40	5	2
1	A	78	GLY	N-CA-C	5.51	118.40	112.33	4	2
1	D	58	VAL	CA-C-O	-5.51	115.33	121.17	13	1
1	C	16	HIS	CA-C-N	5.51	130.00	120.58	6	2
1	C	16	HIS	C-N-CA	5.51	130.00	120.58	6	2
1	B	79	ILE	CA-C-O	-5.51	115.32	121.05	9	1
1	D	31	GLN	O-C-N	5.51	129.23	122.34	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	11	MET	CA-CB-CG	-5.51	103.08	114.10	7	1
1	B	69	ARG	NH1-CZ-NH2	-5.50	112.14	119.30	7	2
1	B	80	ALA	CB-CA-C	5.50	119.92	110.79	2	1
1	A	81	THR	CA-CB-CG2	5.50	119.85	110.50	7	1
1	A	26	LEU	CA-C-O	-5.50	113.64	119.97	7	1
1	B	36	LEU	CA-C-O	-5.50	113.51	118.79	14	1
1	B	18	GLU	CA-C-N	5.50	127.59	120.44	1	2
1	B	18	GLU	C-N-CA	5.50	127.59	120.44	1	2
1	A	90	LYS	N-CA-C	5.50	118.03	111.71	15	1
1	C	27	LYS	CB-CA-C	5.49	120.19	110.85	1	1
1	B	45	PRO	N-CD-CG	5.49	111.44	103.20	3	1
1	A	44	THR	CA-C-O	-5.49	114.72	120.70	5	2
1	D	92	ALA	CB-CA-C	5.49	120.99	110.17	6	1
1	B	15	ARG	CA-C-O	5.49	126.33	120.24	7	1
1	D	58	VAL	CB-CA-C	5.49	119.00	111.97	13	1
1	D	44	THR	CA-CB-OG1	5.49	117.83	109.60	15	1
1	D	22	PHE	N-CA-CB	5.49	118.28	110.16	5	1
1	B	94	VAL	O-C-N	-5.49	114.86	122.05	5	1
1	B	19	TRP	CG-CD2-CE3	-5.49	128.41	133.90	8	1
1	C	81	THR	O-C-N	-5.48	115.53	122.27	15	1
1	D	59	GLU	N-CA-CB	-5.48	102.12	110.07	7	1
1	C	30	TYR	CB-CG-CD1	5.48	129.02	120.80	13	1
1	A	46	ASP	N-CA-C	5.48	119.58	113.01	6	2
1	A	57	ILE	N-CA-C	5.48	115.68	110.42	14	1
1	D	14	GLN	CA-C-N	5.47	131.41	122.65	4	1
1	D	14	GLN	C-N-CA	5.47	131.41	122.65	4	1
1	A	31	GLN	CA-C-N	5.47	130.14	121.44	8	1
1	A	31	GLN	C-N-CA	5.47	130.14	121.44	8	1
1	D	27	LYS	CA-C-O	5.47	126.56	120.82	8	1
1	C	99	TRP	CB-CG-CD2	5.47	134.46	126.80	14	1
1	C	86	SER	CA-C-N	5.47	131.08	122.49	15	1
1	C	86	SER	C-N-CA	5.47	131.08	122.49	15	1
1	B	62	LEU	N-CA-CB	-5.47	102.07	110.44	4	1
1	D	53	THR	OG1-CB-CG2	-5.47	98.36	109.30	7	1
1	A	104	LEU	CA-C-O	5.47	126.31	120.24	9	1
1	D	55	VAL	CA-C-N	5.46	128.05	120.29	6	1
1	D	55	VAL	C-N-CA	5.46	128.05	120.29	6	1
1	D	77	ALA	O-C-N	-5.46	115.23	122.33	14	1
1	D	14	GLN	CA-C-O	-5.46	114.18	120.24	2	1
1	B	21	ARG	CB-CA-C	5.46	119.53	110.90	10	1
1	D	99	TRP	CD2-CE2-CZ2	-5.46	116.94	122.40	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	75	LEU	CA-C-O	-5.46	113.39	119.34	6	1
1	A	45	PRO	N-CA-CB	5.46	108.70	103.52	1	1
1	B	63	ARG	NE-CZ-NH1	5.46	126.96	121.50	1	2
1	C	32	ASN	CA-CB-CG	5.46	118.06	112.60	14	3
1	B	83	THR	CA-CB-CG2	5.46	119.78	110.50	7	1
1	B	23	VAL	N-CA-CB	5.46	120.23	111.23	13	1
1	B	90	LYS	N-CA-C	-5.46	105.23	111.07	5	1
1	A	34	LEU	CB-CA-C	5.46	119.61	110.44	6	1
1	C	85	GLY	N-CA-C	5.45	120.88	112.81	3	1
1	B	103	VAL	CA-CB-CG1	5.45	119.67	110.40	5	1
1	B	86	SER	N-CA-CB	5.45	117.97	110.07	1	1
1	D	89	LEU	CA-C-N	5.45	127.58	120.28	6	2
1	D	89	LEU	C-N-CA	5.45	127.58	120.28	6	2
1	C	99	TRP	CE2-CD2-CG	5.45	113.74	107.20	5	1
1	C	87	ASN	CB-CA-C	5.45	119.19	110.09	13	1
1	C	106	LYS	N-CA-C	5.44	117.75	110.35	5	1
1	C	70	GLU	CA-C-N	5.44	129.31	120.60	15	1
1	C	70	GLU	C-N-CA	5.44	129.31	120.60	15	1
1	C	90	LYS	O-C-N	-5.44	115.54	122.34	13	1
1	A	81	THR	CA-C-O	-5.44	114.78	120.55	4	1
1	B	65	GLU	CB-CG-CD	-5.44	103.36	112.60	5	1
1	D	96	LEU	CA-C-O	-5.44	115.11	120.82	9	1
1	C	70	GLU	CB-CG-CD	-5.43	103.36	112.60	10	1
1	B	50	ALA	N-CA-C	-5.43	105.27	111.14	5	1
1	B	53	THR	N-CA-C	-5.43	104.22	112.04	3	1
1	A	84	ARG	N-CA-CB	-5.43	101.86	110.22	11	1
1	A	20	LEU	N-CA-CB	-5.43	101.86	110.22	12	1
1	D	20	LEU	N-CA-C	5.43	117.20	111.28	15	2
1	B	43	LEU	CA-C-O	-5.42	114.30	120.32	1	1
1	A	106	LYS	CA-C-N	5.42	129.90	120.68	15	1
1	A	106	LYS	C-N-CA	5.42	129.90	120.68	15	1
1	C	40	ASN	O-C-N	-5.42	115.97	122.15	2	1
1	A	13	GLU	CA-C-O	-5.42	115.13	120.82	4	2
1	A	82	ILE	N-CA-CB	5.42	116.77	110.65	6	1
1	B	10	ALA	CB-CA-C	5.42	121.07	110.67	9	1
1	D	89	LEU	CB-CA-C	5.42	119.46	111.17	15	1
1	A	59	GLU	CB-CA-C	5.41	119.38	110.88	5	1
1	C	3	GLN	O-C-N	-5.41	116.91	123.03	6	1
1	A	54	ARG	N-CA-C	5.41	117.18	111.28	6	1
1	C	33	ASP	CA-C-N	5.41	132.12	122.06	10	1
1	C	33	ASP	C-N-CA	5.41	132.12	122.06	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	95	GLU	O-C-N	5.41	129.26	122.23	13	1
1	A	55	VAL	N-CA-CB	5.41	117.89	110.54	13	2
1	B	85	GLY	CA-C-O	-5.40	115.51	120.80	8	1
1	C	15	ARG	O-C-N	-5.40	115.63	122.27	11	1
1	B	82	ILE	N-CA-C	-5.40	105.27	110.72	15	1
1	D	56	ARG	CD-NE-CZ	5.40	131.96	124.40	3	1
1	A	49	GLU	CA-C-O	-5.40	115.14	120.70	10	2
1	A	83	THR	CB-CA-C	5.39	119.35	110.88	4	1
1	A	99	TRP	CG-CD2-CE3	5.39	139.29	133.90	14	2
1	A	89	LEU	CD1-CG-CD2	-5.39	98.93	110.80	8	1
1	D	62	LEU	N-CA-CB	-5.39	102.60	110.47	8	1
1	C	95	GLU	N-CA-C	5.39	118.96	112.38	4	2
1	D	39	LEU	O-C-N	5.39	127.83	122.12	6	1
1	A	65	GLU	CB-CG-CD	5.39	121.76	112.60	7	1
1	D	70	GLU	CB-CG-CD	-5.39	103.44	112.60	7	1
1	C	40	ASN	CB-CG-ND2	5.39	124.48	116.40	11	1
1	A	42	MET	N-CA-CB	-5.39	102.73	110.65	3	1
1	D	25	LEU	CA-C-N	5.39	127.77	120.44	3	1
1	D	25	LEU	C-N-CA	5.39	127.77	120.44	3	1
1	B	63	ARG	CA-C-O	-5.39	115.14	120.80	7	1
1	A	97	ARG	NH1-CZ-NH2	-5.39	112.30	119.30	13	1
1	C	99	TRP	CE2-CD2-CE3	-5.38	113.42	118.80	14	1
1	D	12	ALA	N-CA-C	5.38	117.15	111.28	4	1
1	C	8	SER	CA-C-N	5.38	128.49	120.31	13	2
1	C	8	SER	C-N-CA	5.38	128.49	120.31	13	2
1	C	64	GLY	CA-C-N	5.38	128.49	120.31	11	1
1	C	64	GLY	C-N-CA	5.38	128.49	120.31	11	1
1	C	21	ARG	CD-NE-CZ	5.38	131.93	124.40	13	1
1	C	98	GLN	CA-C-N	5.38	127.75	120.38	5	1
1	C	98	GLN	C-N-CA	5.38	127.75	120.38	5	1
1	C	63	ARG	N-CA-CB	-5.38	102.22	110.01	9	2
1	C	56	ARG	NH1-CZ-NH2	-5.38	112.31	119.30	15	1
1	D	44	THR	OG1-CB-CG2	-5.38	98.55	109.30	14	1
1	C	69	ARG	O-C-N	-5.37	116.03	122.15	12	1
1	B	98	GLN	N-CA-C	-5.37	105.59	111.82	2	1
1	C	59	GLU	CA-C-O	-5.37	114.91	120.92	7	1
1	C	15	ARG	CA-C-N	5.37	127.42	120.44	2	1
1	C	15	ARG	C-N-CA	5.37	127.42	120.44	2	1
1	B	53	THR	CA-C-N	5.37	127.47	120.28	8	2
1	B	53	THR	C-N-CA	5.37	127.47	120.28	8	2
1	B	19	TRP	N-CA-C	5.37	116.81	111.07	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	54	ARG	N-CA-C	5.37	117.88	111.71	14	1
1	C	90	LYS	N-CA-CB	5.36	118.88	110.46	1	1
1	B	45	PRO	CA-C-N	5.36	129.75	120.58	9	1
1	B	45	PRO	C-N-CA	5.36	129.75	120.58	9	1
1	C	49	GLU	O-C-N	-5.36	116.30	122.09	15	1
1	C	66	MET	N-CA-C	5.36	118.00	110.23	15	1
1	A	99	TRP	N-CA-C	5.36	118.15	111.24	5	1
1	B	28	ASN	CB-CG-ND2	5.36	124.44	116.40	13	3
1	C	63	ARG	CA-C-O	5.36	126.23	120.55	11	1
1	B	40	ASN	N-CA-CB	5.36	118.18	110.20	14	1
1	C	85	GLY	O-C-N	-5.36	116.98	122.60	5	1
1	D	69	ARG	O-C-N	-5.35	115.47	122.59	1	1
1	C	105	LEU	CA-C-N	5.35	129.77	121.26	15	1
1	C	105	LEU	C-N-CA	5.35	129.77	121.26	15	1
1	C	93	PRO	CA-N-CD	-5.35	104.51	112.00	11	2
1	A	63	ARG	N-CA-C	5.35	117.19	111.36	12	1
1	B	41	LEU	CB-CA-C	5.35	120.49	110.70	2	1
1	D	35	HIS	ND1-CG-CD2	5.35	111.45	106.10	8	1
1	A	43	LEU	O-C-N	-5.35	116.74	123.27	9	1
1	B	107	SER	CB-CA-C	5.35	120.42	109.67	4	1
1	C	71	LEU	CD1-CG-CD2	-5.35	99.04	110.80	7	1
1	B	66	MET	CB-CG-SD	5.35	128.74	112.70	13	1
1	D	42	MET	O-C-N	-5.35	116.06	122.15	6	1
1	B	39	LEU	CB-CA-C	-5.35	102.26	110.81	8	1
1	C	44	THR	O-C-N	-5.34	115.55	121.53	1	1
1	C	75	LEU	N-CA-CB	5.34	117.81	110.07	6	1
1	B	19	TRP	CA-C-N	5.34	128.43	120.31	12	1
1	B	19	TRP	C-N-CA	5.34	128.43	120.31	12	1
1	D	7	TYR	CB-CG-CD1	-5.34	112.79	120.80	13	1
1	B	84	ARG	NE-CZ-NH2	5.33	124.00	119.20	13	2
1	C	98	GLN	CA-C-O	-5.33	115.19	120.90	10	1
1	D	50	ALA	N-CA-C	5.33	117.17	111.36	15	1
1	A	73	ASN	CB-CG-ND2	5.33	124.40	116.40	12	1
1	A	19	TRP	CG-CD2-CE3	5.33	139.23	133.90	13	1
1	D	27	LYS	CB-CA-C	-5.33	101.94	110.79	2	1
1	D	99	TRP	NE1-CE2-CZ2	5.33	138.09	130.10	3	1
1	B	95	GLU	CA-C-O	-5.33	114.08	120.10	4	1
1	A	24	ASP	CA-C-O	-5.33	115.41	121.00	5	1
1	D	90	LYS	N-CA-CB	-5.33	101.79	110.42	10	1
1	D	40	ASN	CA-C-O	-5.33	113.84	119.97	5	1
1	A	64	GLY	CA-C-O	5.33	125.69	119.19	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	34	LEU	O-C-N	-5.33	113.85	122.42	3	1
1	C	12	ALA	N-CA-CB	-5.32	102.30	110.12	5	1
1	D	85	GLY	CA-C-N	5.32	129.61	120.72	5	1
1	D	85	GLY	C-N-CA	5.32	129.61	120.72	5	1
1	C	66	MET	CA-C-N	5.32	132.42	122.74	6	1
1	C	66	MET	C-N-CA	5.32	132.42	122.74	6	1
1	A	74	GLU	N-CA-C	5.32	117.83	111.71	10	1
1	C	45	PRO	N-CD-CG	5.32	111.18	103.20	11	1
1	D	19	TRP	CG-CD2-CE3	5.32	139.22	133.90	13	1
1	D	49	GLU	N-CA-C	5.32	117.16	111.36	6	2
1	A	56	ARG	NH1-CZ-NH2	-5.32	112.39	119.30	13	3
1	B	17	GLN	CA-C-O	-5.32	113.52	119.79	1	1
1	A	67	SER	CA-C-O	-5.32	115.83	121.94	14	1
1	C	92	ALA	N-CA-C	5.31	117.72	110.01	14	1
1	A	65	GLU	CA-C-O	-5.31	113.67	120.31	8	1
1	A	49	GLU	N-CA-CB	-5.31	102.04	110.22	12	1
1	A	50	ALA	O-C-N	-5.31	116.60	122.07	15	1
1	B	47	GLU	CA-C-N	5.31	127.66	120.44	8	3
1	B	47	GLU	C-N-CA	5.31	127.66	120.44	8	3
1	C	76	GLY	CA-C-N	5.31	131.45	122.26	3	2
1	C	76	GLY	C-N-CA	5.31	131.45	122.26	3	2
1	B	106	LYS	CA-C-N	5.31	131.29	121.52	4	1
1	B	106	LYS	C-N-CA	5.31	131.29	121.52	4	1
1	D	99	TRP	CG-CD2-CE3	-5.31	128.59	133.90	3	1
1	D	71	LEU	O-C-N	-5.31	116.60	122.07	7	1
1	D	45	PRO	N-CD-CG	5.31	111.16	103.20	12	1
1	B	15	ARG	CA-CB-CG	-5.30	103.49	114.10	5	1
1	D	99	TRP	O-C-N	-5.30	116.10	122.15	8	1
1	C	17	GLN	N-CA-C	5.30	119.01	112.54	9	2
1	C	105	LEU	N-CA-CB	-5.30	103.86	111.54	11	1
1	D	92	ALA	O-C-N	-5.29	115.23	121.32	2	1
1	B	49	GLU	N-CA-C	5.29	117.05	111.28	6	1
1	D	52	GLY	CA-C-O	-5.29	115.61	120.80	14	1
1	D	100	LEU	CB-CA-C	-5.29	101.69	110.68	15	1
1	B	73	ASN	N-CA-CB	-5.29	103.56	110.59	7	1
1	A	88	SER	O-C-N	5.29	128.18	122.15	11	2
1	D	69	ARG	CD-NE-CZ	5.29	131.80	124.40	14	1
1	D	54	ARG	N-CA-CB	5.28	118.36	110.22	8	1
1	A	21	ARG	CA-C-O	-5.28	115.28	120.82	1	1
1	B	74	GLU	CA-CB-CG	-5.28	103.54	114.10	11	1
1	B	33	ASP	CA-C-O	5.28	125.43	119.78	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	10	ALA	N-CA-C	-5.28	105.61	111.36	2	1
1	C	77	ALA	CA-C-N	5.28	126.78	120.13	3	2
1	C	77	ALA	C-N-CA	5.28	126.78	120.13	3	2
1	C	90	LYS	CA-C-N	5.28	130.94	121.66	13	1
1	C	90	LYS	C-N-CA	5.28	130.94	121.66	13	1
1	C	44	THR	N-CA-CB	5.28	117.65	110.05	14	1
1	B	68	GLN	N-CA-CB	-5.27	101.37	110.32	2	1
1	D	12	ALA	O-C-N	5.27	128.38	122.22	2	1
1	D	75	LEU	N-CA-CB	5.26	118.27	110.53	2	2
1	D	73	ASN	CA-C-O	-5.26	115.28	120.70	10	1
1	D	34	LEU	CA-C-O	5.26	125.44	119.18	12	1
1	C	86	SER	CA-C-O	-5.26	112.20	119.05	15	1
1	D	97	ARG	O-C-N	5.26	127.70	122.12	15	1
1	D	67	SER	N-CA-CB	-5.26	102.87	110.45	6	2
1	A	18	GLU	CB-CG-CD	-5.26	103.66	112.60	7	1
1	B	104	LEU	CB-CA-C	5.26	119.53	110.86	14	1
1	A	28	ASN	CB-CG-OD1	5.26	131.31	120.80	4	1
1	C	74	GLU	N-CA-C	5.26	118.16	111.69	8	1
1	B	74	GLU	CA-C-N	5.25	130.62	122.26	7	1
1	B	74	GLU	C-N-CA	5.25	130.62	122.26	7	1
1	B	21	ARG	CD-NE-CZ	5.25	131.75	124.40	2	1
1	D	29	ALA	N-CA-CB	-5.25	101.67	110.39	2	1
1	D	32	ASN	CB-CA-C	5.25	118.86	110.09	15	1
1	A	56	ARG	CD-NE-CZ	5.25	131.75	124.40	13	1
1	D	105	LEU	CB-CA-C	5.25	119.58	111.13	15	1
1	B	43	LEU	CA-C-N	5.25	128.66	120.68	1	1
1	B	43	LEU	C-N-CA	5.25	128.66	120.68	1	1
1	D	41	LEU	O-C-N	-5.25	116.17	122.15	7	1
1	D	35	HIS	ND1-CE1-NE2	5.24	113.64	108.40	1	1
1	B	20	LEU	CA-C-O	-5.24	113.15	119.49	2	1
1	A	16	HIS	CA-C-O	-5.24	115.32	120.82	1	1
1	C	58	VAL	CA-C-O	-5.24	115.50	120.95	10	1
1	B	97	ARG	NE-CZ-NH1	-5.24	116.27	121.50	10	2
1	C	38	LEU	N-CA-C	5.24	116.99	111.28	12	1
1	C	73	ASN	CB-CG-ND2	5.24	124.25	116.40	13	1
1	B	48	ARG	CA-C-O	-5.23	115.01	120.55	2	1
1	C	73	ASN	CA-C-O	-5.23	112.96	119.18	12	1
1	D	106	LYS	CB-CG-CD	5.23	123.32	111.30	12	1
1	A	99	TRP	NE1-CE2-CZ2	5.22	137.94	130.10	5	1
1	C	24	ASP	CA-CB-CG	5.22	117.83	112.60	13	1
1	A	13	GLU	O-C-N	-5.22	116.20	122.15	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	100	LEU	N-CA-C	5.22	117.38	111.11	9	1
1	D	96	LEU	CD1-CG-CD2	-5.22	99.31	110.80	9	1
1	B	32	ASN	CA-C-N	5.22	129.54	122.19	4	1
1	B	32	ASN	C-N-CA	5.22	129.54	122.19	4	1
1	B	19	TRP	N-CA-CB	-5.21	102.45	110.01	7	1
1	B	34	LEU	O-C-N	-5.21	115.44	122.22	13	1
1	C	32	ASN	N-CA-CB	-5.21	103.27	111.39	5	1
1	C	36	LEU	CA-C-O	-5.20	113.03	120.16	10	2
1	B	86	SER	CA-C-N	5.20	127.56	120.54	1	2
1	B	86	SER	C-N-CA	5.20	127.56	120.54	1	2
1	D	67	SER	O-C-N	-5.20	116.60	122.68	1	1
1	B	51	LEU	CA-C-N	5.20	126.64	120.14	3	3
1	B	51	LEU	C-N-CA	5.20	126.64	120.14	3	3
1	B	79	ILE	O-C-N	-5.20	116.80	121.89	3	1
1	C	19	TRP	O-C-N	-5.20	116.61	122.12	14	1
1	B	98	GLN	O-C-N	-5.19	115.88	122.27	2	1
1	B	80	ALA	CA-C-N	5.19	129.38	120.71	13	1
1	B	80	ALA	C-N-CA	5.19	129.38	120.71	13	1
1	B	37	PRO	CA-C-N	5.19	127.19	120.44	1	1
1	B	37	PRO	C-N-CA	5.19	127.19	120.44	1	1
1	D	81	THR	OG1-CB-CG2	-5.18	98.93	109.30	2	1
1	D	22	PHE	CA-C-N	5.18	127.09	120.56	5	1
1	D	22	PHE	C-N-CA	5.18	127.09	120.56	5	1
1	C	9	ALA	CA-C-N	5.18	129.37	120.72	8	1
1	C	9	ALA	C-N-CA	5.18	129.37	120.72	8	1
1	D	57	ILE	CA-CB-CG1	5.18	119.20	110.40	12	1
1	D	107	SER	O-C-N	-5.18	116.30	122.20	13	1
1	A	29	ALA	CA-C-N	5.18	127.22	120.28	1	1
1	A	29	ALA	C-N-CA	5.18	127.22	120.28	1	1
1	D	51	LEU	CA-C-O	-5.17	115.06	120.55	1	1
1	B	104	LEU	CD1-CG-CD2	-5.17	99.42	110.80	2	2
1	B	53	THR	N-CA-CB	5.17	117.51	110.01	14	2
1	C	27	LYS	N-CA-CB	-5.17	102.51	110.16	1	1
1	D	94	VAL	CA-CB-CG1	5.17	119.19	110.40	8	1
1	D	15	ARG	CA-C-O	-5.17	115.07	120.55	11	2
1	A	99	TRP	CB-CG-CD1	-5.17	119.15	126.90	13	1
1	B	97	ARG	CA-C-O	-5.17	114.03	119.97	2	1
1	A	58	VAL	CA-C-O	-5.17	115.04	120.57	4	1
1	B	79	ILE	CA-CB-CG2	5.17	119.28	110.50	9	1
1	A	86	SER	CA-C-N	5.16	129.41	120.58	1	2
1	A	86	SER	C-N-CA	5.16	129.41	120.58	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	22	PHE	O-C-N	-5.16	116.65	122.12	5	1
1	A	104	LEU	CB-CG-CD2	5.16	126.19	110.70	6	1
1	A	22	PHE	N-CA-CB	-5.16	102.51	110.20	12	1
1	B	85	GLY	N-CA-C	5.16	118.93	112.73	14	1
1	C	31	GLN	CA-C-N	5.16	132.89	123.13	9	1
1	C	31	GLN	C-N-CA	5.16	132.89	123.13	9	1
1	A	32	ASN	CA-CB-CG	-5.16	107.44	112.60	7	1
1	B	94	VAL	CA-CB-CG1	5.16	119.17	110.40	13	1
1	B	19	TRP	CE2-CD2-CE3	-5.16	113.64	118.80	14	1
1	C	31	GLN	O-C-N	-5.16	115.53	122.23	5	1
1	C	17	GLN	CB-CA-C	5.15	119.34	110.79	2	1
1	C	42	MET	CA-C-N	5.15	130.67	122.94	13	2
1	C	42	MET	C-N-CA	5.15	130.67	122.94	13	2
1	C	96	LEU	CA-C-O	-5.15	115.59	120.90	5	1
1	A	52	GLY	CA-C-O	-5.15	115.44	121.00	14	1
1	A	11	MET	CB-CA-C	5.15	120.12	110.70	13	1
1	B	106	LYS	CA-C-O	-5.15	112.52	119.11	13	1
1	A	26	LEU	O-C-N	-5.15	116.33	122.20	14	1
1	D	41	LEU	N-CA-CB	-5.15	102.54	110.16	2	1
1	D	9	ALA	N-CA-CB	-5.15	101.57	110.32	4	1
1	A	62	LEU	O-C-N	-5.15	116.53	122.09	5	1
1	B	41	LEU	N-CA-CB	-5.15	102.54	110.16	7	2
1	A	89	LEU	O-C-N	-5.14	115.94	122.27	6	1
1	D	10	ALA	N-CA-C	-5.14	105.59	111.14	7	1
1	C	89	LEU	CA-C-O	5.14	126.18	120.63	7	1
1	A	94	VAL	CA-CB-CG2	5.14	119.14	110.40	15	2
1	C	5	SER	CA-C-N	5.14	125.59	120.04	9	1
1	C	5	SER	C-N-CA	5.14	125.59	120.04	9	1
1	A	99	TRP	O-C-N	-5.13	115.37	122.30	10	1
1	C	26	LEU	N-CA-C	-5.13	105.60	111.14	2	1
1	D	86	SER	CA-C-N	5.13	131.34	121.54	9	1
1	D	86	SER	C-N-CA	5.13	131.34	121.54	9	1
1	B	89	LEU	CA-C-N	5.13	127.11	120.44	13	1
1	B	89	LEU	C-N-CA	5.13	127.11	120.44	13	1
1	C	94	VAL	CG1-CB-CG2	-5.13	99.52	110.80	9	1
1	B	74	GLU	O-C-N	-5.13	116.04	122.35	12	1
1	A	11	MET	CA-C-N	5.12	127.66	120.28	3	1
1	A	11	MET	C-N-CA	5.12	127.66	120.28	3	1
1	D	83	THR	CA-C-O	-5.12	113.31	119.15	9	1
1	B	62	LEU	CD1-CG-CD2	-5.12	99.53	110.80	12	1
1	A	21	ARG	O-C-N	5.12	127.35	122.07	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	43	LEU	N-CA-C	5.12	117.84	109.59	8	1
1	A	97	ARG	CD-NE-CZ	5.12	131.57	124.40	9	1
1	A	44	THR	OG1-CB-CG2	-5.12	99.06	109.30	8	1
1	C	36	LEU	N-CA-CB	5.12	116.46	110.42	2	1
1	D	96	LEU	CB-CA-C	5.12	119.00	110.81	6	1
1	C	8	SER	CA-C-O	5.12	125.67	120.24	12	1
1	C	38	LEU	O-C-N	5.12	127.55	122.12	12	1
1	C	103	VAL	N-CA-C	-5.12	106.69	111.45	15	1
1	A	19	TRP	CB-CA-C	5.12	118.98	110.90	5	1
1	A	37	PRO	N-CD-CG	5.11	110.87	103.20	3	1
1	D	18	GLU	CA-CB-CG	-5.11	103.88	114.10	6	1
1	B	68	GLN	N-CA-C	5.11	116.85	111.28	5	1
1	D	91	ALA	CB-CA-C	5.11	117.99	109.56	4	1
1	D	78	GLY	CA-C-N	5.11	131.16	121.97	7	2
1	D	78	GLY	C-N-CA	5.11	131.16	121.97	7	2
1	D	37	PRO	CA-C-N	5.11	129.31	120.58	9	1
1	D	37	PRO	C-N-CA	5.11	129.31	120.58	9	1
1	D	27	LYS	N-CA-C	5.11	117.25	111.02	7	1
1	B	80	ALA	N-CA-CB	-5.10	102.60	110.20	3	1
1	B	25	LEU	CA-C-O	5.10	126.17	120.82	3	1
1	D	10	ALA	CB-CA-C	5.10	118.96	110.90	3	1
1	B	94	VAL	N-CA-CB	5.10	117.47	110.54	4	1
1	D	19	TRP	CE2-CD2-CE3	-5.10	113.70	118.80	11	1
1	A	51	LEU	CD1-CG-CD2	-5.10	99.59	110.80	3	1
1	A	88	SER	CA-C-O	-5.10	115.02	120.42	2	1
1	A	100	LEU	O-C-N	-5.10	116.26	122.22	14	1
1	C	102	GLU	N-CA-C	-5.09	106.57	112.89	4	1
1	D	61	LEU	CA-C-N	5.09	127.52	120.29	4	1
1	D	61	LEU	C-N-CA	5.09	127.52	120.29	4	1
1	A	35	HIS	CE1-NE2-CD2	5.09	114.09	109.00	10	1
1	D	40	ASN	CB-CG-ND2	5.09	124.03	116.40	13	1
1	A	74	GLU	CA-C-N	5.09	130.35	122.26	1	1
1	A	74	GLU	C-N-CA	5.09	130.35	122.26	1	1
1	B	38	LEU	CB-CA-C	5.09	119.33	110.79	8	1
1	C	26	LEU	CD1-CG-CD2	-5.09	99.61	110.80	9	2
1	C	23	VAL	O-C-N	5.08	126.89	121.91	7	1
1	D	46	ASP	N-CA-CB	5.08	118.69	110.40	9	1
1	D	21	ARG	NE-CZ-NH1	5.08	126.58	121.50	3	1
1	B	82	ILE	CA-CB-CG1	5.08	119.04	110.40	11	1
1	A	14	GLN	CA-C-N	5.08	128.73	120.60	15	1
1	A	14	GLN	C-N-CA	5.08	128.73	120.60	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	46	ASP	O-C-N	5.08	127.50	122.12	6	1
1	B	46	ASP	CA-C-N	5.08	127.08	120.28	1	1
1	B	46	ASP	C-N-CA	5.08	127.08	120.28	1	1
1	C	51	LEU	N-CA-CB	-5.08	102.40	110.22	5	1
1	A	76	GLY	O-C-N	-5.08	115.89	122.34	6	1
1	B	82	ILE	CA-C-O	-5.08	115.28	120.71	8	2
1	D	84	ARG	CA-C-O	-5.08	116.10	121.94	8	1
1	A	69	ARG	CA-C-N	5.07	127.50	120.29	8	1
1	A	69	ARG	C-N-CA	5.07	127.50	120.29	8	1
1	A	89	LEU	CB-CA-C	5.07	118.92	110.90	14	2
1	D	103	VAL	O-C-N	-5.07	116.61	122.04	11	1
1	D	107	SER	CA-C-N	5.07	130.83	121.70	14	1
1	D	107	SER	C-N-CA	5.07	130.83	121.70	14	1
1	A	69	ARG	NH1-CZ-NH2	-5.07	112.71	119.30	6	1
1	C	98	GLN	N-CA-C	5.07	117.54	111.71	7	1
1	B	19	TRP	CB-CG-CD2	5.07	133.90	126.80	8	1
1	A	14	GLN	CA-CB-CG	-5.07	103.96	114.10	15	1
1	B	11	MET	CA-C-O	-5.07	113.81	119.79	1	2
1	D	55	VAL	CA-CB-CG2	5.07	119.02	110.40	1	1
1	C	66	MET	O-C-N	-5.07	117.29	123.27	10	1
1	D	28	ASN	CA-C-N	5.07	127.48	120.29	15	1
1	D	28	ASN	C-N-CA	5.07	127.48	120.29	15	1
1	B	27	LYS	CA-C-O	5.06	126.32	120.90	3	1
1	B	55	VAL	N-CA-C	5.06	115.28	110.42	4	1
1	B	87	ASN	N-CA-CB	-5.06	102.68	110.12	4	1
1	C	28	ASN	CA-C-O	5.06	125.79	120.42	7	2
1	A	45	PRO	N-CD-CG	5.06	110.79	103.20	12	1
1	C	90	LYS	CA-CB-CG	-5.06	103.98	114.10	13	1
1	C	53	THR	OG1-CB-CG2	-5.06	99.18	109.30	9	1
1	C	17	GLN	CG-CD-NE2	5.06	123.99	116.40	5	1
1	B	70	GLU	N-CA-C	5.06	116.80	111.28	7	1
1	B	71	LEU	N-CA-C	5.06	117.45	111.33	12	1
1	A	58	VAL	CA-C-N	5.06	127.82	120.79	2	1
1	A	58	VAL	C-N-CA	5.06	127.82	120.79	2	1
1	C	21	ARG	CB-CG-CD	-5.06	99.67	111.30	1	1
1	D	99	TRP	CG-CD1-NE1	-5.06	103.63	110.20	3	1
1	B	25	LEU	O-C-N	-5.05	116.86	122.07	3	1
1	A	60	GLU	N-CA-CB	5.05	118.08	110.30	6	1
1	D	94	VAL	CB-CA-C	-5.05	104.33	112.16	14	1
1	B	38	LEU	CA-C-N	5.05	129.16	120.72	15	1
1	B	38	LEU	C-N-CA	5.05	129.16	120.72	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	TRP	CE2-CD2-CG	5.05	113.26	107.20	10	1
1	C	59	GLU	N-CA-C	5.05	117.44	111.33	3	1
1	B	10	ALA	CA-C-O	-5.05	115.07	120.42	6	1
1	B	89	LEU	N-CA-C	5.05	116.47	111.07	6	1
1	A	23	VAL	CA-C-N	5.05	127.00	120.44	8	1
1	A	23	VAL	C-N-CA	5.05	127.00	120.44	8	1
1	B	94	VAL	N-CA-C	5.05	117.36	111.05	10	1
1	C	64	GLY	N-CA-C	5.05	122.67	114.90	3	1
1	C	56	ARG	CD-NE-CZ	5.05	131.47	124.40	12	1
1	C	1	MET	CB-CA-C	5.05	119.69	110.10	15	1
1	D	56	ARG	CA-CB-CG	5.04	124.19	114.10	5	1
1	A	64	GLY	CA-C-N	5.04	129.25	120.68	10	1
1	A	64	GLY	C-N-CA	5.04	129.25	120.68	10	1
1	A	43	LEU	CB-CA-C	5.04	118.94	109.71	14	1
1	A	32	ASN	CB-CA-C	5.04	119.24	110.72	5	1
1	A	40	ASN	CB-CG-ND2	5.04	123.95	116.40	9	1
1	B	59	GLU	CA-C-N	5.04	129.95	121.14	5	1
1	B	59	GLU	C-N-CA	5.04	129.95	121.14	5	1
1	B	45	PRO	N-CA-C	5.04	121.11	113.81	8	1
1	C	56	ARG	N-CA-C	5.04	118.57	112.23	8	1
1	C	26	LEU	CA-C-N	5.04	127.79	120.79	11	1
1	C	26	LEU	C-N-CA	5.04	127.79	120.79	11	1
1	B	87	ASN	CB-CG-ND2	5.03	123.95	116.40	6	1
1	D	33	ASP	CA-C-O	-5.03	114.53	120.57	9	1
1	D	19	TRP	N-CA-CB	-5.03	102.76	110.26	10	1
1	A	93	PRO	O-C-N	-5.03	116.87	123.06	3	1
1	B	27	LYS	O-C-N	5.03	127.45	122.12	8	1
1	A	45	PRO	CA-C-N	5.03	129.12	120.72	13	1
1	A	45	PRO	C-N-CA	5.03	129.12	120.72	13	1
1	B	12	ALA	N-CA-CB	5.03	117.51	110.12	1	1
1	B	16	HIS	CA-C-O	-5.03	115.52	120.90	7	1
1	D	47	GLU	CA-C-O	-5.03	114.19	119.97	8	1
1	D	57	ILE	N-CA-C	-5.03	105.80	110.53	5	1
1	D	38	LEU	N-CA-C	5.03	116.57	111.14	3	1
1	C	62	LEU	CB-CA-C	5.03	118.77	110.88	9	1
1	D	21	ARG	N-CA-C	-5.02	105.71	111.14	4	1
1	C	56	ARG	O-C-N	-5.02	115.60	122.33	13	1
1	B	97	ARG	N-CA-C	5.02	116.83	111.36	5	2
1	B	13	GLU	CA-CB-CG	5.02	124.14	114.10	4	1
1	A	61	LEU	CA-C-O	-5.02	113.09	119.31	14	1
1	C	37	PRO	N-CD-CG	5.02	110.73	103.20	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	18	GLU	CA-C-O	5.02	126.09	120.82	15	1
1	A	99	TRP	CD2-CE2-CZ2	-5.01	117.39	122.40	5	1
1	D	95	GLU	CA-C-O	-5.01	114.04	120.31	12	1
1	A	45	PRO	CA-N-CD	-5.01	104.98	112.00	7	1
1	B	104	LEU	CA-C-N	5.01	127.49	120.28	2	1
1	B	104	LEU	C-N-CA	5.01	127.49	120.28	2	1
1	A	75	LEU	CA-C-O	5.01	124.41	118.90	2	1
1	B	67	SER	CA-C-O	-5.01	116.06	121.87	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	D	92	ALA	Peptide	12
1	B	48	ARG	Sidechain	7
1	B	30	TYR	Sidechain	6
1	D	54	ARG	Sidechain,Mainchain	6
1	D	21	ARG	Sidechain,Peptide	5
1	B	15	ARG	Sidechain,Peptide	5
1	D	56	ARG	Sidechain	4
1	A	97	ARG	Sidechain,Mainchain	4
1	C	54	ARG	Sidechain	4
1	D	30	TYR	Sidechain	4
1	D	69	ARG	Peptide,Sidechain	4
1	A	21	ARG	Sidechain	4
1	D	15	ARG	Peptide,Sidechain	4
1	D	91	ALA	Peptide	4
1	C	7	TYR	Sidechain	3
1	B	63	ARG	Sidechain	3
1	C	63	ARG	Sidechain	3
1	A	48	ARG	Sidechain	3
1	D	84	ARG	Sidechain,Peptide	3
1	D	48	ARG	Sidechain	3
1	D	75	LEU	Peptide,Mainchain	3
1	D	85	GLY	Peptide	3
1	B	97	ARG	Sidechain	3
1	B	84	ARG	Sidechain	3
1	A	54	ARG	Sidechain	2
1	C	21	ARG	Sidechain	2
1	A	23	VAL	Mainchain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	52	GLY	Mainchain	2
1	D	6	PRO	Peptide	2
1	C	15	ARG	Sidechain	2
1	C	97	ARG	Sidechain	2
1	A	22	PHE	Sidechain	2
1	B	16	HIS	Mainchain,Sidechain	2
1	D	80	ALA	Mainchain,Peptide	2
1	A	15	ARG	Mainchain,Sidechain	2
1	D	22	PHE	Mainchain,Sidechain	2
1	C	16	HIS	Sidechain,Mainchain	2
1	B	69	ARG	Sidechain	2
1	D	83	THR	Mainchain,Peptide	2
1	A	69	ARG	Sidechain	2
1	C	84	ARG	Sidechain	2
1	B	54	ARG	Mainchain	1
1	C	52	GLY	Mainchain	1
1	A	27	LYS	Mainchain	1
1	B	24	ASP	Sidechain	1
1	C	48	ARG	Sidechain	1
1	A	62	LEU	Peptide	1
1	D	94	VAL	Mainchain	1
1	D	102	GLU	Mainchain	1
1	A	103	VAL	Mainchain	1
1	B	22	PHE	Sidechain	1
1	B	74	GLU	Mainchain	1
1	D	51	LEU	Peptide	1
1	A	96	LEU	Mainchain	1
1	B	86	SER	Mainchain	1
1	C	91	ALA	Peptide	1
1	D	65	GLU	Peptide	1
1	D	76	GLY	Peptide	1
1	A	63	ARG	Sidechain	1
1	C	30	TYR	Sidechain	1
1	D	79	ILE	Mainchain	1
1	A	35	HIS	Sidechain	1
1	D	31	GLN	Mainchain	1
1	D	95	GLU	Peptide	1
1	A	79	ILE	Mainchain	1
1	C	88	SER	Peptide	1
1	C	94	VAL	Mainchain	1
1	B	68	GLN	Mainchain	1
1	C	80	ALA	Mainchain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	D	7	TYR	Sidechain	1
1	D	9	ALA	Mainchain	1
1	A	30	TYR	Sidechain	1
1	A	104	LEU	Peptide	1
1	C	76	GLY	Mainchain	1
1	D	36	LEU	Mainchain	1
1	A	94	VAL	Mainchain	1
1	B	94	VAL	Mainchain	1
1	C	33	ASP	Sidechain	1
1	C	56	ARG	Sidechain	1
1	D	90	LYS	Mainchain	1
1	A	26	LEU	Mainchain	1
1	B	35	HIS	Sidechain	1
1	B	95	GLU	Mainchain	1
1	D	66	MET	Peptide	1
1	D	78	GLY	Mainchain	1
1	A	25	LEU	Mainchain	1
1	B	21	ARG	Sidechain	1
1	B	83	THR	Mainchain	1
1	C	69	ARG	Sidechain	1
1	D	89	LEU	Peptide	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	D	836	848	848	2±1
1	A	780	803	803	0±0
1	B	800	817	817	0±1
1	C	852	871	871	1±1
All	All	49020	50085	50085	34

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:D:92:ALA:HA	1:D:93:PRO:C	0.59	2.23	5	7
1:C:19:TRP:CZ2	1:D:48:ARG:HD2	0.56	2.36	9	2
1:D:92:ALA:HB1	1:D:94:VAL:HG22	0.53	1.81	6	1
1:C:39:LEU:HD13	1:D:19:TRP:CZ2	0.53	2.39	3	1
1:B:44:THR:HB	1:B:45:PRO:CD	0.52	2.35	6	1
1:C:39:LEU:HD13	1:D:19:TRP:CH2	0.50	2.42	3	1
1:D:93:PRO:HA	1:D:95:GLU:OE2	0.49	2.08	14	3
1:C:32:ASN:HD21	1:D:99:TRP:CD1	0.47	2.27	3	1
1:B:44:THR:HB	1:B:45:PRO:HD2	0.47	1.87	7	1
1:A:22:PHE:CE1	1:A:26:LEU:HD22	0.47	2.44	13	1
1:D:29:ALA:HB1	1:D:35:HIS:HA	0.47	1.87	6	1
1:D:26:LEU:O	1:D:29:ALA:HB3	0.47	2.09	10	1
1:D:19:TRP:CZ3	1:D:22:PHE:CD1	0.46	3.04	10	1
1:D:75:LEU:HD22	1:D:75:LEU:N	0.44	2.28	5	1
1:A:30:TYR:CD1	1:A:35:HIS:CG	0.43	3.06	11	1
1:A:30:TYR:CE1	1:A:35:HIS:CD2	0.43	3.06	7	1
1:D:92:ALA:C	1:D:94:VAL:N	0.42	2.76	10	1
1:C:81:THR:HG23	1:D:44:THR:HG23	0.42	1.90	2	1
1:D:92:ALA:HA	1:D:94:VAL:N	0.41	2.31	15	1
1:C:66:MET:HA	1:C:66:MET:HE2	0.41	1.92	12	1
1:D:93:PRO:C	1:D:95:GLU:H	0.41	2.23	2	1
1:A:58:VAL:HG21	1:B:42:MET:HE1	0.40	1.91	6	1
1:C:51:LEU:HD13	1:D:22:PHE:CE1	0.40	2.50	7	1
1:C:22:PHE:CD1	1:C:22:PHE:C	0.40	2.99	14	1
1:C:19:TRP:CZ2	1:D:39:LEU:HD13	0.40	2.52	12	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/108 (89%)	94±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	49	83
1	B	98/108 (91%)	95±2 (97±2%)	3±1 (3±1%)	0±0 (0±0%)	49	83
1	C	105/108 (97%)	101±1 (96±1%)	3±1 (3±1%)	0±0 (0±0%)	37	78
1	D	103/108 (95%)	93±2 (91±2%)	7±2 (7±2%)	2±1 (2±1%)	7	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6030/6480 (93%)	5748 (95%)	237 (4%)	45 (1%)	20 70

All 15 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	D	93	PRO	15
1	D	68	GLN	7
1	D	92	ALA	5
1	C	88	SER	3
1	D	77	ALA	3
1	D	94	VAL	2
1	D	35	HIS	2
1	A	67	SER	1
1	C	92	ALA	1
1	D	6	PRO	1
1	B	64	GLY	1
1	D	78	GLY	1
1	D	79	ILE	1
1	A	33	ASP	1
1	C	64	GLY	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	84/93 (90%)	83±1 (99±2%)	1±1 (1±2%)	57 93
1	B	86/93 (92%)	85±1 (99±1%)	1±1 (1±1%)	59 94
1	C	91/93 (98%)	89±1 (97±1%)	2±1 (3±1%)	40 87
1	D	90/93 (97%)	84±2 (93±2%)	6±2 (7±2%)	15 63
All	All	5265/5580 (94%)	5096 (97%)	169 (3%)	35 84

All 55 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	C	15	ARG	15
1	D	95	GLU	15
1	D	15	ARG	14
1	D	35	HIS	13
1	D	71	LEU	10
1	D	89	LEU	8
1	C	46	ASP	7
1	D	75	LEU	5
1	D	46	ASP	4
1	D	79	ILE	4
1	A	17	GLN	4
1	D	93	PRO	4
1	C	33	ASP	4
1	A	46	ASP	3
1	B	46	ASP	3
1	D	108	ASP	3
1	B	89	LEU	3
1	D	45	PRO	3
1	D	36	LEU	3
1	B	33	ASP	2
1	D	11	MET	2
1	C	20	LEU	2
1	D	33	ASP	2
1	D	107	SER	2
1	A	41	LEU	2
1	B	11	MET	2
1	A	94	VAL	2
1	B	32	ASN	1
1	C	69	ARG	1
1	C	94	VAL	1
1	D	94	VAL	1
1	A	81	THR	1
1	C	37	PRO	1
1	C	75	LEU	1
1	C	30	TYR	1
1	A	24	ASP	1
1	D	37	PRO	1
1	B	60	GLU	1
1	B	61	LEU	1
1	B	94	VAL	1
1	C	45	PRO	1
1	A	11	MET	1
1	A	83	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	C	42	MET	1
1	B	16	HIS	1
1	D	19	TRP	1
1	D	42	MET	1
1	C	24	ASP	1
1	C	74	GLU	1
1	A	53	THR	1
1	B	18	GLU	1
1	A	19	TRP	1
1	A	37	PRO	1
1	B	37	PRO	1
1	D	8	SER	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 11% for the well-defined parts and 12% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	725
Number of shifts mapped to atoms	725
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	103	-2.12 ± 0.25	Should be checked
$^{13}\text{C}_\beta$	81	0.89 ± 0.19	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	88	0.92 ± 0.57	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 11%, i.e. 649 atoms were assigned a chemical shift out of a possible 5835. 0 out of 96 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	338/2017 (17%)	169/816 (21%)	91/810 (11%)	78/391 (20%)
Sidechain	307/3572 (9%)	207/2317 (9%)	100/1089 (9%)	0/166 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	4/246 (2%)	2/124 (2%)	0/106 (0%)	2/16 (12%)
Overall	649/5835 (11%)	378/3257 (12%)	191/2005 (10%)	80/573 (14%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 12%, i.e. 725 atoms were assigned a chemical shift out of a possible 6148. 0 out of 96 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	379/2148 (18%)	188/868 (22%)	103/864 (12%)	88/416 (21%)
Sidechain	342/3736 (9%)	227/2424 (9%)	115/1140 (10%)	0/172 (0%)
Aromatic	4/264 (2%)	2/132 (2%)	0/116 (0%)	2/16 (12%)
Overall	725/6148 (12%)	417/3424 (12%)	218/2120 (10%)	90/604 (15%)

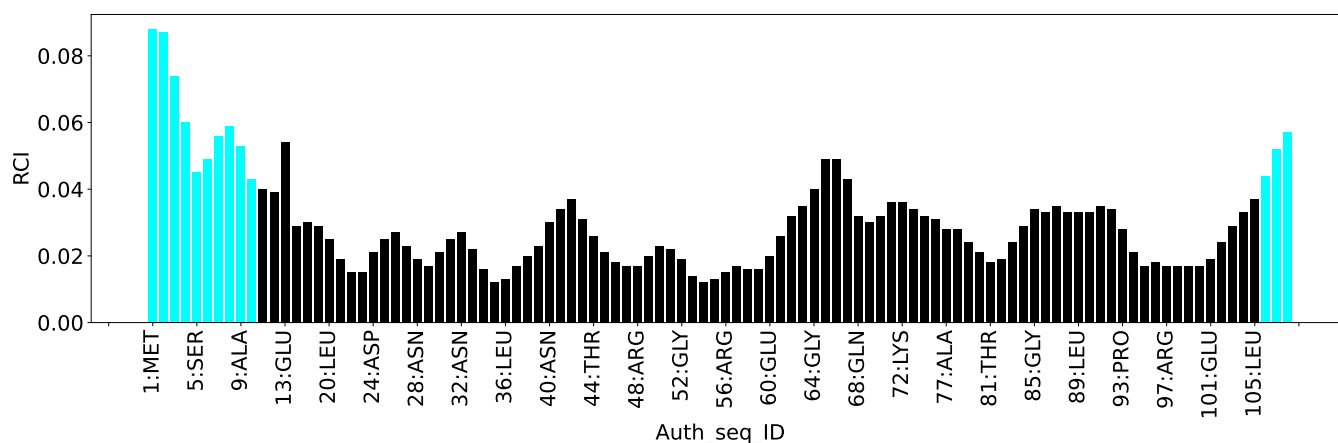
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1084
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	471
Medium range ($ i-j >1$ and $ i-j <5$)	523
Long range ($ i-j \geq 5$)	90
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	2.5
Number of long range restraints per residue ¹	0.2

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)	31.5	0.2
0.2-0.5 (Medium)	54.4	0.5
>0.5 (Large)	154.2	9.44

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 ⓘ

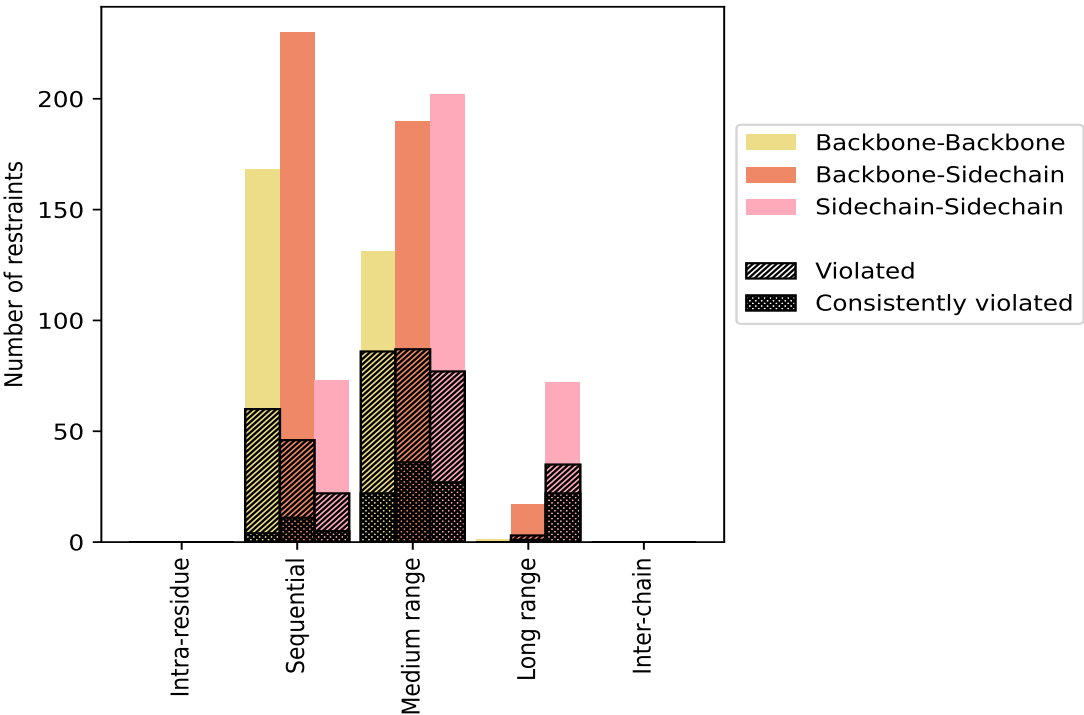
9.1 Summary of distance violations ⓘ

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$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	471	43.5	128	27.2	11.8	20	4.2	1.8
Backbone-Backbone	168	15.5	60	35.7	5.5	4	2.4	0.4
Backbone-Sidechain	230	21.2	46	20.0	4.2	11	4.8	1.0
Sidechain-Sidechain	73	6.7	22	30.1	2.0	5	6.8	0.5
Medium range ($ i-j >1$ & $ i-j <5$)	523	48.2	250	47.8	23.1	85	16.3	7.8
Backbone-Backbone	131	12.1	86	65.6	7.9	22	16.8	2.0
Backbone-Sidechain	190	17.5	87	45.8	8.0	36	18.9	3.3
Sidechain-Sidechain	202	18.6	77	38.1	7.1	27	13.4	2.5
Long range ($ i-j \geq 5$)	90	8.3	38	42.2	3.5	23	25.6	2.1
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	17	1.6	3	17.6	0.3	1	5.9	0.1
Sidechain-Sidechain	72	6.6	35	48.6	3.2	22	30.6	2.0
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	1084	100.0	416	38.4	38.4	128	11.8	11.8
Backbone-Backbone	300	27.7	146	48.7	13.5	26	8.7	2.4
Backbone-Sidechain	437	40.3	136	31.1	12.5	48	11.0	4.4
Sidechain-Sidechain	347	32.0	134	38.6	12.4	54	15.6	5.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	59	152	27	0	238	1.46	8.6	1.75	0.71
2	0	62	144	27	0	233	1.44	8.83	1.7	0.82
3	0	57	149	28	0	234	1.45	9.28	1.77	0.77
4	0	63	147	28	0	238	1.37	7.6	1.55	0.79
5	0	62	146	29	0	237	1.41	8.47	1.61	0.82
6	0	59	148	26	0	233	1.5	8.77	1.7	0.89
7	0	64	159	27	0	250	1.38	8.59	1.61	0.8
8	0	62	149	27	0	238	1.34	8.45	1.52	0.84
9	0	62	166	28	0	256	1.29	8.62	1.55	0.76
10	0	65	146	32	0	243	1.33	7.89	1.55	0.78

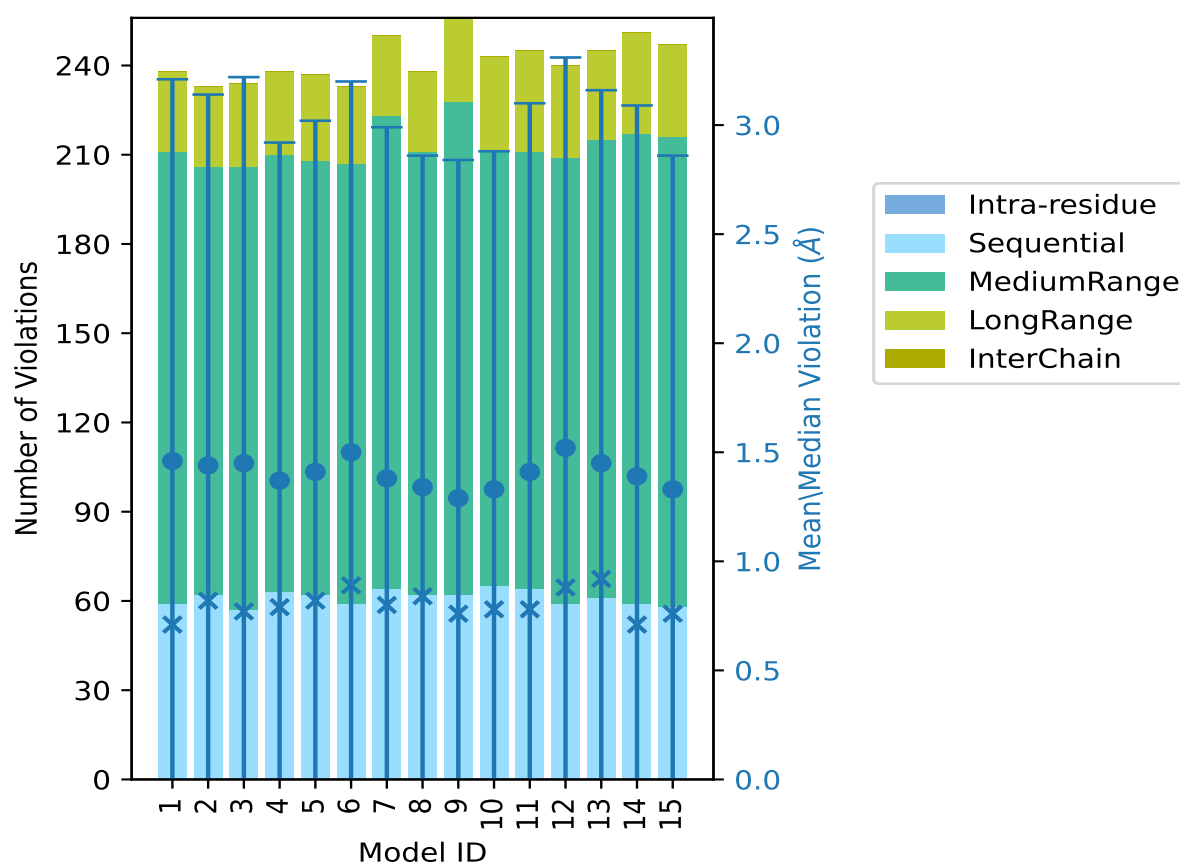
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	64	147	34	0	245	1.41	8.74	1.69	0.78
12	0	59	150	31	0	240	1.52	9.21	1.79	0.88
13	0	61	154	30	0	245	1.45	9.44	1.71	0.92
14	0	59	158	34	0	251	1.39	8.72	1.7	0.71
15	0	58	158	31	0	247	1.33	7.82	1.53	0.76

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

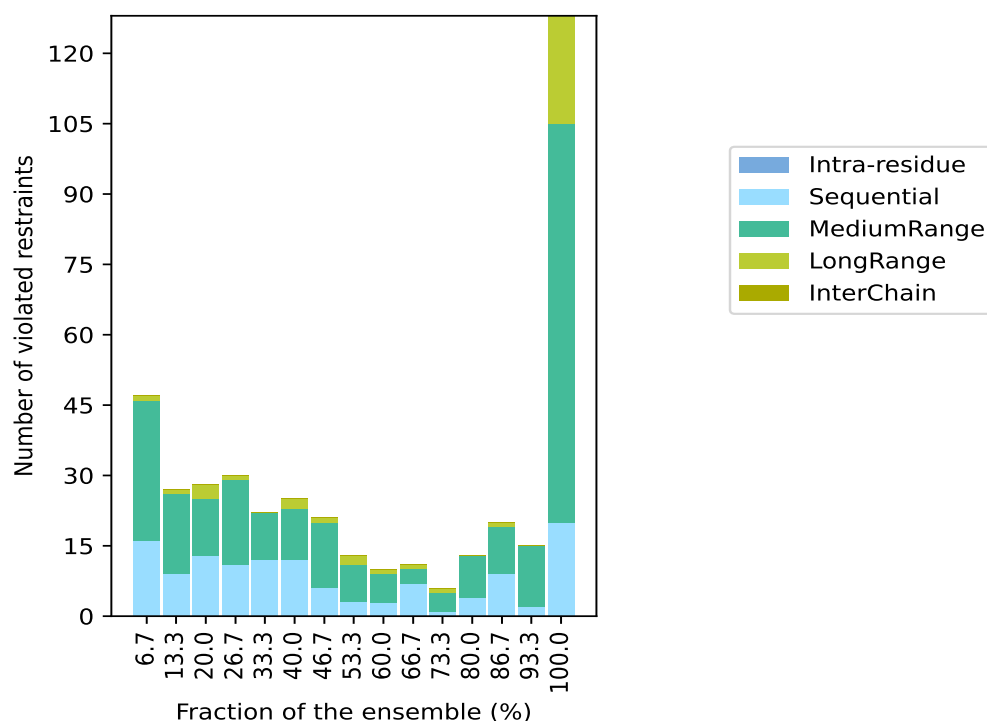
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 668(IR:0, SQ:343, MR:273, LR:52, IC:0) restraints are not 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	%
0	16	30	1	0	47	1	6.7
0	9	17	1	0	27	2	13.3
0	13	12	3	0	28	3	20.0
0	11	18	1	0	30	4	26.7
0	12	10	0	0	22	5	33.3
0	12	11	2	0	25	6	40.0
0	6	14	1	0	21	7	46.7
0	3	8	2	0	13	8	53.3
0	3	6	1	0	10	9	60.0
0	7	3	1	0	11	10	66.7
0	1	4	1	0	6	11	73.3
0	4	9	0	0	13	12	80.0
0	9	10	1	0	20	13	86.7
0	2	13	0	0	15	14	93.3
0	20	85	23	0	128	15	100.0

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

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

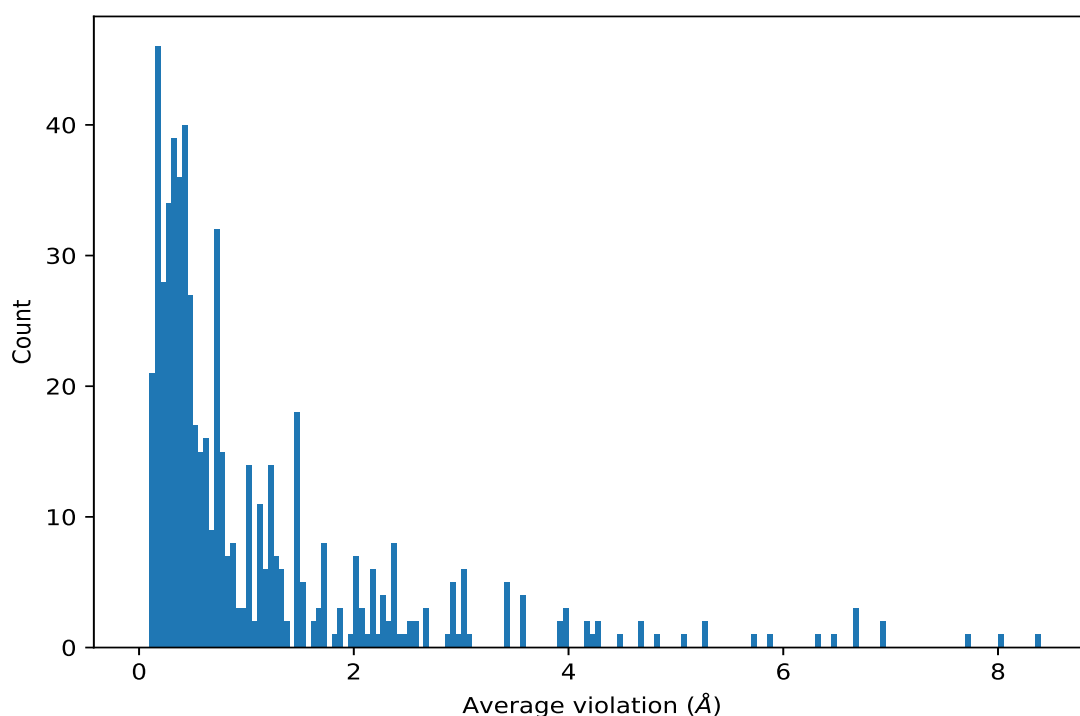
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	15	8.37	0.53	8.55
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	15	8.0	0.66	8.16
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	15	7.74	0.62	7.6
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	15	6.91	0.69	6.82
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	15	6.91	0.69	6.82
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	15	6.67	1.01	6.43
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	15	6.66	0.83	6.61
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	15	6.66	0.83	6.61
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	15	6.45	0.95	6.24
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	15	6.3	1.12	6.21
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	15	5.85	0.86	5.89
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	15	5.7	0.37	5.68
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	15	5.25	1.1	4.93
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	15	5.25	1.1	4.93
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	15	5.06	0.36	5.03
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	15	4.83	1.04	4.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	15	4.68	0.98	4.76
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	15	4.68	0.98	4.76
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	15	4.48	0.92	4.68
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	15	4.29	0.31	4.24
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	15	4.29	0.31	4.24
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	15	4.24	0.21	4.26
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	15	4.19	1.08	4.18
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	15	4.16	0.98	4.4
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	15	3.95	0.37	3.91
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	15	3.95	0.37	3.91
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	15	3.95	0.37	3.91
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	15	3.93	0.39	3.89
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	15	3.93	0.39	3.89
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	15	3.58	0.56	3.61
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	15	3.58	0.56	3.61
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	15	3.58	0.56	3.61
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	15	3.57	0.28	3.53
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	15	3.43	0.5	3.3
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	15	3.43	0.5	3.3
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	15	3.43	0.5	3.3
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	15	3.43	0.5	3.3
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	15	3.43	0.5	3.3
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	15	3.09	0.24	3.09
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	15	3.03	0.6	2.94
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	15	3.03	0.6	2.94
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	15	3.03	0.6	2.94
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	15	3.03	0.6	2.94
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	15	3.03	0.6	2.94
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	15	3.02	0.48	3.25
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	15	2.99	0.84	3.19
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	15	2.92	0.07	2.92
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	15	2.9	1.07	2.68
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	15	2.9	1.07	2.68
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	15	2.9	1.07	2.68
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	15	2.9	1.07	2.68
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	15	2.86	0.55	3.08
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	15	2.69	0.37	2.7
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	15	2.66	1.19	3.04
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	15	2.66	1.19	3.04
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	15	2.56	0.22	2.58
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	15	2.56	0.22	2.58
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	15	2.54	0.52	2.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	15	2.54	0.52	2.57
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	15	2.47	0.32	2.55
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	15	2.41	0.63	2.31
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	15	2.39	1.26	2.26
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	15	2.39	1.26	2.26
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	15	2.39	1.26	2.26
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	15	2.39	1.26	2.26
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	15	2.39	1.26	2.26
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	15	2.39	1.26	2.26
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	15	2.36	0.31	2.44
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	15	2.36	0.31	2.44
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	15	2.34	0.33	2.32
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	15	2.34	0.33	2.32
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	15	2.28	0.43	2.23
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	15	2.25	0.97	2.04
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	15	2.25	0.97	2.04
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	15	2.25	0.97	2.04
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	15	2.22	0.47	2.22
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	15	2.18	0.68	2.29
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	15	2.18	0.68	2.29
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	15	2.18	0.68	2.29
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	15	2.18	0.34	2.28
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	15	2.18	0.34	2.28
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	15	2.17	0.69	2.42
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	15	2.1	0.46	2.16
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	15	2.05	0.33	2.05
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	15	2.05	0.33	2.05
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	15	2.05	0.33	2.05
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	15	2.04	0.2	1.97
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	15	2.04	0.2	1.97
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	15	2.0	0.39	2.03
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	15	2.0	0.39	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	15	2.0	0.39	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	15	2.0	0.39	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	15	2.0	0.39	2.03
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	15	1.98	0.25	2.07
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	15	1.89	0.92	2.45
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	15	1.85	0.24	1.96
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	15	1.82	0.64	1.71
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	15	1.73	0.15	1.75
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	15	1.73	0.15	1.75
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	15	1.73	0.92	2.03

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	15	1.73	0.92	2.03
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	15	1.73	0.92	2.03
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	15	1.7	0.25	1.74
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	15	1.7	0.25	1.74
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	15	1.7	0.25	1.74
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	15	1.69	0.21	1.69
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	15	1.69	0.21	1.69
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	15	1.68	0.25	1.72
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	15	1.63	0.75	1.23
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	15	1.6	0.54	1.61
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	15	1.54	0.68	1.86
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	15	1.52	0.37	1.48
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	15	1.52	0.37	1.48
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	15	1.52	0.37	1.48
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	15	1.52	0.46	1.54
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	15	1.49	0.23	1.48
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	15	1.49	0.23	1.48
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	15	1.49	0.23	1.48
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	15	1.49	0.23	1.48
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	15	1.49	0.23	1.48
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	15	1.48	0.41	1.55
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	15	1.48	0.41	1.55
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	15	1.48	0.41	1.55
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	15	1.48	0.69	1.52
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	15	1.48	0.69	1.52
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	15	1.48	0.69	1.52
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	15	1.48	0.69	1.52
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	15	1.48	0.69	1.52
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	15	1.47	0.29	1.45
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	15	1.47	0.29	1.45
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	15	1.47	0.29	1.45
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	15	1.46	0.55	1.59
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	15	1.46	0.55	1.59
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	15	1.39	0.43	1.44
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	15	1.34	0.33	1.41
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	15	1.34	0.19	1.34
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	15	1.34	0.35	1.28
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	15	1.3	0.32	1.26
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	15	1.3	0.32	1.26
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	15	1.3	0.32	1.26
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	15	1.29	0.27	1.16
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	15	1.29	0.27	1.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	15	1.29	0.53	1.29
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	15	1.28	0.57	1.23
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	15	1.26	0.27	1.28
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	15	1.25	0.16	1.2
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	15	1.23	0.21	1.24
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	15	1.22	0.4	1.15
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	15	1.21	0.13	1.2
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	15	1.19	0.37	1.14
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	15	1.19	0.37	1.14
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	15	1.19	0.37	1.14
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	15	1.17	0.33	1.17
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	15	1.14	0.11	1.15
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	15	1.14	0.11	1.15
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	15	1.11	0.12	1.08
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	15	1.11	0.12	1.08
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	15	1.11	0.53	1.18
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	15	1.1	0.33	1.06
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	15	1.1	0.33	1.06
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	15	1.1	0.33	1.06
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	15	1.1	0.33	1.06
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	15	1.1	0.33	1.06
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	15	1.04	0.46	1.11
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	15	1.03	0.32	1.04
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	15	1.02	0.52	1.05
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	15	1.02	0.58	1.01
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	15	1.01	0.23	0.93
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	15	1.01	0.23	0.93
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	15	1.01	0.23	0.93
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	15	0.94	0.19	0.92
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	15	0.9	0.22	0.93
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	15	0.89	0.39	0.92
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	15	0.87	0.19	0.9
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	15	0.87	0.21	0.91
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	15	0.87	0.21	0.91
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	15	0.85	0.44	0.9
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	15	0.85	0.29	0.97
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	15	0.83	0.27	0.8
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	15	0.82	0.3	0.82
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	15	0.8	0.25	0.78
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	15	0.77	0.21	0.81
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	15	0.76	0.19	0.75
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	15	0.76	0.19	0.75

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	15	0.76	0.19	0.75
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	15	0.76	0.19	0.75
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	15	0.76	0.19	0.75
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	15	0.76	0.19	0.75
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	15	0.76	0.22	0.76
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	15	0.75	0.2	0.84
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	15	0.74	0.29	0.85
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	15	0.74	0.29	0.85
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	15	0.73	0.23	0.73
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	15	0.73	0.23	0.73
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	15	0.73	0.23	0.73
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	15	0.71	0.24	0.77
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	15	0.71	0.24	0.77
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	15	0.71	0.24	0.77
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	15	0.7	0.25	0.64
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	15	0.67	0.3	0.68
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	15	0.67	0.29	0.73
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	15	0.66	0.2	0.63
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	15	0.65	0.26	0.63
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	15	0.63	0.26	0.67
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	15	0.63	0.16	0.67
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	15	0.62	0.34	0.6
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	15	0.62	0.34	0.6
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	15	0.61	0.21	0.53
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	15	0.59	0.25	0.59
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	15	0.53	0.23	0.49
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	15	0.53	0.25	0.51
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	15	0.5	0.27	0.45
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	15	0.5	0.27	0.45
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	15	0.41	0.19	0.34
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	15	0.41	0.19	0.34
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	15	0.31	0.07	0.33
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	15	0.28	0.09	0.27
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	14	1.28	0.57	1.05
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	14	1.2	0.62	1.44
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	14	1.2	0.62	1.44
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	14	1.2	0.62	1.44
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	14	1.2	0.62	1.44
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	14	1.2	0.62	1.44
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	14	1.2	0.62	1.44
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	14	1.2	0.62	1.44
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	14	1.2	0.62	1.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	14	1.2	0.62	1.44
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	14	0.97	0.29	1.0
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	14	0.97	0.29	1.0
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	14	0.97	0.29	1.0
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	14	0.8	0.23	0.8
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	14	0.8	0.23	0.8
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	14	0.8	0.23	0.8
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	14	0.7	0.27	0.71
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	14	0.7	0.27	0.71
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	14	0.7	0.27	0.71
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	14	0.7	0.27	0.71
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	14	0.7	0.27	0.71
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	14	0.7	0.27	0.71
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	14	0.67	0.25	0.68
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	14	0.63	0.35	0.61
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	14	0.59	0.22	0.6
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	14	0.51	0.27	0.54
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	14	0.46	0.24	0.42
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	14	0.45	0.17	0.4
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	14	0.45	0.19	0.48
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	14	0.45	0.19	0.48
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	14	0.45	0.19	0.48
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	14	0.43	0.15	0.41
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	14	0.43	0.15	0.41
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	14	0.41	0.23	0.36
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	14	0.41	0.23	0.36
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	14	0.41	0.23	0.36
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	14	0.41	0.23	0.36
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	14	0.41	0.23	0.36
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	14	0.32	0.09	0.3
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	13	1.21	0.2	1.21
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	13	1.17	0.34	1.25
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	13	1.16	0.55	1.24
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	13	1.08	0.46	1.0
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	13	1.03	0.35	1.11
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	13	1.03	0.35	1.11
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	13	1.03	0.35	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	13	1.03	0.35	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	13	1.03	0.35	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	13	1.03	0.35	1.11
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	13	0.87	0.47	0.89
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	13	0.75	0.4	0.84

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	13	0.71	0.37	0.62
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	13	0.71	0.37	0.62
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	13	0.64	0.23	0.69
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	13	0.64	0.23	0.69
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	13	0.63	0.25	0.64
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	13	0.63	0.25	0.64
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	13	0.63	0.25	0.64
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	13	0.63	0.25	0.64
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	13	0.63	0.25	0.64
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	13	0.63	0.25	0.64
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	13	0.54	0.29	0.44
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	13	0.54	0.29	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	13	0.53	0.15	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	13	0.53	0.15	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	13	0.53	0.15	0.44
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	13	0.48	0.2	0.48
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	13	0.46	0.3	0.46
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	13	0.46	0.3	0.46
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	13	0.46	0.3	0.46
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	13	0.46	0.3	0.46
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	13	0.42	0.17	0.36
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	13	0.32	0.12	0.33
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	13	0.32	0.12	0.33
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	13	0.32	0.12	0.33
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	13	0.3	0.08	0.31
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	13	0.26	0.1	0.25
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	13	0.26	0.08	0.28
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	13	0.26	0.08	0.28
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	13	0.26	0.05	0.26
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	12	0.89	0.34	0.8
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	12	0.72	0.52	0.56
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	12	0.72	0.52	0.56
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	12	0.72	0.52	0.56
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	12	0.5	0.33	0.41
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	12	0.5	0.33	0.41
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	12	0.49	0.21	0.44
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	12	0.44	0.19	0.42
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	12	0.44	0.22	0.36
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	12	0.43	0.21	0.38
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	12	0.42	0.21	0.4
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	12	0.42	0.21	0.4
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	12	0.39	0.2	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	12	0.38	0.17	0.34
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	12	0.36	0.16	0.37
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	12	0.32	0.11	0.31
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	12	0.28	0.09	0.26
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	11	1.23	0.37	1.4
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	11	1.01	0.58	1.01
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	11	0.78	0.32	0.73
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	11	0.41	0.26	0.33
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	11	0.41	0.26	0.33
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	11	0.38	0.18	0.31
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	11	0.38	0.18	0.31
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	11	0.37	0.18	0.29
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	11	0.37	0.18	0.29
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG21	10	0.7	0.32	0.64
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG21	10	0.7	0.32	0.64
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG21	10	0.7	0.32	0.64
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG22	10	0.7	0.32	0.64
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG22	10	0.7	0.32	0.64
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG22	10	0.7	0.32	0.64
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG23	10	0.7	0.32	0.64
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG23	10	0.7	0.32	0.64
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG23	10	0.7	0.32	0.64
(1,400)	1:41:A:LEU:HD21	1:42:A:MET:H	10	0.6	0.31	0.54
(1,66)	1:19:A:TRP:HA	1:23:A:VAL:H	10	0.52	0.31	0.5
(1,69)	1:19:A:TRP:H	1:20:A:LEU:HG	10	0.44	0.2	0.41
(1,19)	1:15:A:ARG:HG3	1:19:A:TRP:H	10	0.44	0.19	0.37
(1,19)	1:15:A:ARG:HG2	1:19:A:TRP:H	10	0.44	0.19	0.37
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD11	10	0.43	0.08	0.42
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD12	10	0.43	0.08	0.42
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD13	10	0.43	0.08	0.42
(1,76)	1:20:A:LEU:HD21	1:21:A:ARG:H	10	0.41	0.39	0.3
(1,441)	1:47:A:GLU:HA	1:49:A:GLU:H	10	0.38	0.17	0.28
(1,546)	1:56:A:ARG:HG3	1:57:A:ILE:HA	10	0.36	0.08	0.34
(1,546)	1:56:A:ARG:HG2	1:57:A:ILE:HA	10	0.36	0.08	0.34
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD22	10	0.3	0.14	0.26
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD23	10	0.3	0.14	0.26
(1,294)	1:35:A:HIS:HA	1:36:A:LEU:H	10	0.15	0.05	0.12
(1,602)	1:58:A:VAL:HG21	1:96:A:LEU:HD21	9	1.85	0.61	1.84
(1,721)	1:67:A:SER:HA	1:71:A:LEU:HD21	9	0.9	0.32	0.94
(1,210)	1:27:A:LYS:HD3	1:28:A:ASN:H	9	0.67	0.21	0.7
(1,210)	1:27:A:LYS:HD2	1:28:A:ASN:H	9	0.67	0.21	0.7
(1,945)	1:96:A:LEU:HD22	1:100:A:LEU:HD21	9	0.47	0.2	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,384)	1:39:A:LEU:HD21	1:40:A:ASN:H	9	0.4	0.11	0.41
(1,786)	1:78:A:GLY:H	1:81:A:THR:H	9	0.39	0.18	0.45
(1,353)	1:37:A:PRO:HA	1:40:A:ASN:H	9	0.37	0.15	0.39
(1,693)	1:64:A:GLY:HA3	1:66:A:MET:HA	9	0.3	0.11	0.34
(1,693)	1:64:A:GLY:HA2	1:66:A:MET:HA	9	0.3	0.11	0.34
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD22	9	0.27	0.14	0.19
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD23	9	0.27	0.14	0.19
(1,486)	1:51:A:LEU:HD11	1:54:A:ARG:H	9	0.23	0.11	0.19
(1,486)	1:51:A:LEU:HD12	1:54:A:ARG:H	9	0.23	0.11	0.19
(1,486)	1:51:A:LEU:HD13	1:54:A:ARG:H	9	0.23	0.11	0.19
(1,606)	1:58:A:VAL:HG23	1:96:A:LEU:HD21	8	1.38	0.67	1.32
(1,598)	1:58:A:VAL:HG12	1:96:A:LEU:HD21	8	1.08	0.49	1.28
(1,982)	1:100:A:LEU:HD21	1:102:A:GLU:H	8	0.78	0.36	0.82
(1,588)	1:58:A:VAL:HG21	1:61:A:LEU:HD21	8	0.73	0.53	0.73
(1,1026)	1:103:A:VAL:H	1:104:A:LEU:HD21	8	0.49	0.19	0.48
(1,84)	1:20:A:LEU:HD11	1:23:A:VAL:HG11	8	0.44	0.36	0.2
(1,84)	1:20:A:LEU:HD12	1:23:A:VAL:HG11	8	0.44	0.36	0.2
(1,84)	1:20:A:LEU:HD13	1:23:A:VAL:HG11	8	0.44	0.36	0.2
(1,933)	1:96:A:LEU:HD22	1:99:A:TRP:HB2	8	0.35	0.17	0.34
(1,933)	1:96:A:LEU:HD23	1:99:A:TRP:HB2	8	0.35	0.17	0.34
(1,965)	1:98:A:GLN:HA	1:101:A:GLU:H	8	0.35	0.16	0.29
(1,980)	1:100:A:LEU:HD22	1:101:A:GLU:H	8	0.3	0.07	0.3
(1,980)	1:100:A:LEU:HD23	1:101:A:GLU:H	8	0.3	0.07	0.3
(1,172)	1:25:A:LEU:HA	1:28:A:ASN:H	8	0.29	0.12	0.26
(1,717)	1:67:A:SER:HA	1:70:A:GLU:H	8	0.26	0.11	0.24
(1,191)	1:26:A:LEU:HA	1:29:A:ALA:H	8	0.19	0.04	0.18
(1,553)	1:57:A:ILE:HA	1:58:A:VAL:H	8	0.18	0.04	0.18
(1,328)	1:36:A:LEU:HD21	1:39:A:LEU:HD21	7	0.82	0.74	0.25
(1,942)	1:96:A:LEU:HD21	1:100:A:LEU:HD21	7	0.59	0.4	0.5
(1,563)	1:57:A:ILE:HG23	1:61:A:LEU:HD21	7	0.56	0.27	0.43
(1,329)	1:36:A:LEU:HD22	1:39:A:LEU:HD21	7	0.55	0.2	0.56
(1,329)	1:36:A:LEU:HD23	1:39:A:LEU:HD21	7	0.55	0.2	0.56
(1,586)	1:58:A:VAL:HG13	1:61:A:LEU:HD21	7	0.55	0.29	0.56
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD22	7	0.54	0.24	0.56
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD23	7	0.54	0.24	0.56
(1,860)	1:89:A:LEU:HD21	1:92:A:ALA:HB1	7	0.47	0.24	0.52
(1,1083)	1:106:A:LYS:HG3	1:108:A:ASP:H	7	0.45	0.21	0.3
(1,1083)	1:106:A:LYS:HG2	1:108:A:ASP:H	7	0.45	0.21	0.3
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD22	7	0.42	0.21	0.4
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD23	7	0.42	0.21	0.4
(1,223)	1:28:A:ASN:HA	1:32:A:ASN:H	7	0.38	0.16	0.43
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD22	7	0.34	0.22	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD23	7	0.34	0.22	0.24
(1,675)	1:62:A:LEU:HD11	1:64:A:GLY:H	7	0.34	0.16	0.24
(1,675)	1:62:A:LEU:HD12	1:64:A:GLY:H	7	0.34	0.16	0.24
(1,675)	1:62:A:LEU:HD13	1:64:A:GLY:H	7	0.34	0.16	0.24
(1,181)	1:25:A:LEU:HD22	1:28:A:ASN:HB2	7	0.33	0.2	0.31
(1,181)	1:25:A:LEU:HD23	1:28:A:ASN:HB2	7	0.33	0.2	0.31
(1,748)	1:71:A:LEU:HD21	1:72:A:LYS:H	7	0.32	0.07	0.34
(1,632)	1:59:A:GLU:HG2	1:104:A:LEU:HD21	7	0.3	0.15	0.25
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG11	7	0.26	0.08	0.26
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG12	7	0.26	0.08	0.26
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG13	7	0.26	0.08	0.26
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG21	7	0.26	0.08	0.26
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG22	7	0.26	0.08	0.26
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG23	7	0.26	0.08	0.26
(1,459)	1:50:A:ALA:HA	1:51:A:LEU:H	7	0.19	0.07	0.17
(1,1028)	1:103:A:VAL:HA	1:104:A:LEU:H	7	0.15	0.05	0.13
(1,454)	1:49:A:GLU:HA	1:50:A:ALA:H	7	0.15	0.03	0.16
(1,968)	1:99:A:TRP:HA	1:100:A:LEU:H	7	0.14	0.03	0.14
(1,361)	1:38:A:LEU:HA	1:39:A:LEU:H	7	0.14	0.01	0.14
(1,600)	1:58:A:VAL:HG13	1:96:A:LEU:HD21	6	0.78	0.39	0.87
(1,604)	1:58:A:VAL:HG22	1:96:A:LEU:HD21	6	0.68	0.4	0.76
(1,864)	1:89:A:LEU:HD21	1:92:A:ALA:HB3	6	0.57	0.3	0.4
(1,462)	1:50:A:ALA:HB1	1:51:A:LEU:HD21	6	0.56	0.15	0.6
(1,974)	1:99:A:TRP:HA	1:103:A:VAL:H	6	0.55	0.46	0.31
(1,405)	1:42:A:MET:H	1:43:A:LEU:HG	6	0.54	0.33	0.58
(1,333)	1:36:A:LEU:HD21	1:39:A:LEU:HD23	6	0.52	0.27	0.52
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG3	6	0.48	0.16	0.5
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG2	6	0.48	0.16	0.5
(1,559)	1:57:A:ILE:HG21	1:61:A:LEU:HD21	6	0.46	0.22	0.43
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD22	6	0.39	0.14	0.42
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD23	6	0.39	0.14	0.42
(1,142)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	6	0.38	0.24	0.38
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD22	6	0.36	0.15	0.3
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD23	6	0.36	0.15	0.3
(1,201)	1:26:A:LEU:HG	1:30:A:TYR:H	6	0.32	0.15	0.32
(1,1008)	1:101:A:GLU:HA	1:105:A:LEU:H	6	0.31	0.28	0.18
(1,64)	1:19:A:TRP:HA	1:22:A:PHE:H	6	0.31	0.13	0.28
(1,278)	1:33:A:ASP:H	1:34:A:LEU:HG	6	0.25	0.08	0.24
(1,1070)	1:104:A:LEU:HD22	1:106:A:LYS:H	6	0.24	0.08	0.22
(1,1070)	1:104:A:LEU:HD23	1:106:A:LYS:H	6	0.24	0.08	0.22
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD11	6	0.2	0.07	0.18
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD12	6	0.2	0.07	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD13	6	0.2	0.07	0.18
(1,824)	1:87:A:ASN:HA	1:88:A:SER:H	6	0.18	0.05	0.16
(1,157)	1:24:A:ASP:HA	1:25:A:LEU:H	6	0.18	0.05	0.18
(1,226)	1:29:A:ALA:HA	1:30:A:TYR:H	6	0.18	0.08	0.13
(1,535)	1:55:A:VAL:HA	1:56:A:ARG:H	6	0.16	0.04	0.15
(1,831)	1:88:A:SER:HA	1:89:A:LEU:H	6	0.16	0.04	0.16
(1,976)	1:100:A:LEU:HA	1:101:A:GLU:H	6	0.16	0.03	0.16
(1,649)	1:61:A:LEU:HA	1:62:A:LEU:H	6	0.15	0.02	0.14
(1,491)	1:51:A:LEU:HD22	1:54:A:ARG:HA	5	0.71	0.36	0.66
(1,491)	1:51:A:LEU:HD23	1:54:A:ARG:HA	5	0.71	0.36	0.66
(1,947)	1:96:A:LEU:HD23	1:100:A:LEU:HD21	5	0.44	0.14	0.44
(1,71)	1:19:A:TRP:H	1:20:A:LEU:HD21	5	0.37	0.33	0.14
(1,13)	1:12:A:ALA:HA	1:15:A:ARG:H	5	0.31	0.09	0.34
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD22	5	0.3	0.16	0.32
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD23	5	0.3	0.16	0.32
(1,103)	1:21:A:ARG:HA	1:24:A:ASP:H	5	0.29	0.07	0.3
(1,298)	1:35:A:HIS:HA	1:38:A:LEU:H	5	0.29	0.09	0.26
(1,492)	1:51:A:LEU:HD11	1:54:A:ARG:HD3	5	0.28	0.08	0.33
(1,492)	1:51:A:LEU:HD12	1:54:A:ARG:HD3	5	0.28	0.08	0.33
(1,492)	1:51:A:LEU:HD13	1:54:A:ARG:HD3	5	0.28	0.08	0.33
(1,144)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	5	0.24	0.1	0.2
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB3	5	0.22	0.07	0.19
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB2	5	0.22	0.07	0.19
(1,158)	1:24:A:ASP:HA	1:27:A:LYS:H	5	0.2	0.09	0.18
(1,924)	1:96:A:LEU:HD22	1:98:A:GLN:H	5	0.19	0.11	0.13
(1,924)	1:96:A:LEU:HD23	1:98:A:GLN:H	5	0.19	0.11	0.13
(1,197)	1:26:A:LEU:HD21	1:29:A:ALA:HB2	5	0.19	0.09	0.16
(1,8)	1:11:A:MET:HA	1:12:A:ALA:H	5	0.18	0.05	0.17
(1,98)	1:21:A:ARG:H	1:22:A:PHE:H	5	0.17	0.05	0.18
(1,695)	1:65:A:GLU:HA	1:66:A:MET:H	5	0.17	0.04	0.16
(1,167)	1:25:A:LEU:HA	1:26:A:LEU:H	5	0.16	0.02	0.16
(1,398)	1:41:A:LEU:HA	1:42:A:MET:H	5	0.15	0.04	0.15
(1,762)	1:73:A:ASN:HA	1:74:A:GLU:H	5	0.14	0.03	0.13
(1,243)	1:30:A:TYR:HA	1:31:A:GLN:H	5	0.14	0.02	0.14
(1,735)	1:70:A:GLU:HA	1:71:A:LEU:H	5	0.14	0.02	0.14
(1,40)	1:18:A:GLU:HA	1:19:A:TRP:H	5	0.13	0.02	0.13
(1,707)	1:66:A:MET:HB3	1:68:A:GLN:HB3	4	0.57	0.26	0.52
(1,707)	1:66:A:MET:HB3	1:68:A:GLN:HB2	4	0.57	0.26	0.52
(1,707)	1:66:A:MET:HB2	1:68:A:GLN:HB3	4	0.57	0.26	0.52
(1,707)	1:66:A:MET:HB2	1:68:A:GLN:HB2	4	0.57	0.26	0.52
(1,895)	1:93:A:PRO:HG3	1:97:A:ARG:H	4	0.48	0.21	0.5
(1,895)	1:93:A:PRO:HG2	1:97:A:ARG:H	4	0.48	0.21	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,509)	1:51:A:LEU:HD21	1:55:A:VAL:HG23	4	0.46	0.15	0.48
(1,1022)	1:102:A:GLU:HA	1:106:A:LYS:H	4	0.46	0.16	0.43
(1,487)	1:51:A:LEU:HD21	1:54:A:ARG:H	4	0.45	0.15	0.48
(1,960)	1:97:A:ARG:HA	1:101:A:GLU:HB3	4	0.39	0.16	0.39
(1,960)	1:97:A:ARG:HA	1:101:A:GLU:HB2	4	0.39	0.16	0.39
(1,983)	1:100:A:LEU:HD22	1:102:A:GLU:H	4	0.38	0.13	0.4
(1,983)	1:100:A:LEU:HD23	1:102:A:GLU:H	4	0.38	0.13	0.4
(1,1020)	1:102:A:GLU:HA	1:105:A:LEU:H	4	0.38	0.14	0.4
(1,217)	1:27:A:LYS:HA	1:31:A:GLN:H	4	0.37	0.15	0.31
(1,272)	1:32:A:ASN:HB2	1:34:A:LEU:HD21	4	0.35	0.19	0.3
(1,523)	1:53:A:THR:HA	1:57:A:ILE:H	4	0.35	0.13	0.3
(1,435)	1:46:A:ASP:HA	1:49:A:GLU:H	4	0.34	0.15	0.34
(1,394)	1:40:A:ASN:H	1:41:A:LEU:HD22	4	0.32	0.14	0.28
(1,394)	1:40:A:ASN:H	1:41:A:LEU:HD23	4	0.32	0.14	0.28
(1,215)	1:27:A:LYS:HA	1:30:A:TYR:H	4	0.32	0.17	0.3
(1,174)	1:25:A:LEU:HD11	1:28:A:ASN:HA	4	0.27	0.15	0.2
(1,174)	1:25:A:LEU:HD12	1:28:A:ASN:HA	4	0.27	0.15	0.2
(1,174)	1:25:A:LEU:HD13	1:28:A:ASN:HA	4	0.27	0.15	0.2
(1,114)	1:22:A:PHE:HA	1:25:A:LEU:H	4	0.27	0.13	0.24
(1,972)	1:99:A:TRP:HA	1:102:A:GLU:H	4	0.26	0.12	0.24
(1,107)	1:21:A:ARG:HB3	1:25:A:LEU:HD21	4	0.24	0.06	0.23
(1,421)	1:43:A:LEU:HD22	1:48:A:ARG:HD2	4	0.22	0.1	0.18
(1,421)	1:43:A:LEU:HD23	1:48:A:ARG:HD2	4	0.22	0.1	0.18
(1,366)	1:38:A:LEU:HA	1:41:A:LEU:H	4	0.22	0.12	0.17
(1,437)	1:47:A:GLU:H	1:48:A:ARG:HB3	4	0.21	0.08	0.2
(1,437)	1:47:A:GLU:H	1:48:A:ARG:HB2	4	0.21	0.08	0.2
(1,674)	1:62:A:LEU:HG	1:63:A:ARG:H	4	0.19	0.09	0.15
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD11	4	0.18	0.04	0.16
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD12	4	0.18	0.04	0.16
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD13	4	0.18	0.04	0.16
(1,892)	1:93:A:PRO:HG3	1:94:A:VAL:H	4	0.16	0.03	0.16
(1,892)	1:93:A:PRO:HG2	1:94:A:VAL:H	4	0.16	0.03	0.16
(1,738)	1:70:A:GLU:HG3	1:71:A:LEU:HB3	4	0.16	0.02	0.16
(1,738)	1:70:A:GLU:HG3	1:71:A:LEU:HB2	4	0.16	0.02	0.16
(1,738)	1:70:A:GLU:HG2	1:71:A:LEU:HB3	4	0.16	0.02	0.16
(1,738)	1:70:A:GLU:HG2	1:71:A:LEU:HB2	4	0.16	0.02	0.16
(1,10)	1:12:A:ALA:HA	1:13:A:GLU:H	4	0.15	0.04	0.15
(1,1014)	1:102:A:GLU:HA	1:103:A:VAL:H	4	0.14	0.03	0.14
(1,219)	1:28:A:ASN:HA	1:29:A:ALA:H	4	0.14	0.02	0.14
(1,126)	1:23:A:VAL:HA	1:24:A:ASP:H	4	0.13	0.03	0.12
(1,380)	1:39:A:LEU:HA	1:40:A:ASN:H	4	0.12	0.02	0.12
(1,331)	1:36:A:LEU:HD21	1:39:A:LEU:HD22	3	1.1	0.16	1.05

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,801)	1:81:A:THR:HA	1:84:A:ARG:H	3	0.47	0.22	0.43
(1,1012)	1:101:A:GLU:HA	1:105:A:LEU:HD22	3	0.47	0.05	0.5
(1,1012)	1:101:A:GLU:HA	1:105:A:LEU:HD23	3	0.47	0.05	0.5
(1,497)	1:51:A:LEU:HA	1:55:A:VAL:H	3	0.44	0.18	0.46
(1,722)	1:67:A:SER:HA	1:71:A:LEU:HD22	3	0.43	0.23	0.4
(1,722)	1:67:A:SER:HA	1:71:A:LEU:HD23	3	0.43	0.23	0.4
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD11	3	0.41	0.09	0.38
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD12	3	0.41	0.09	0.38
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD13	3	0.41	0.09	0.38
(1,117)	1:22:A:PHE:HB3	1:25:A:LEU:HD21	3	0.41	0.1	0.44
(1,248)	1:30:A:TYR:HE1	1:39:A:LEU:HD21	3	0.36	0.07	0.32
(1,372)	1:38:A:LEU:HA	1:41:A:LEU:HD22	3	0.35	0.13	0.4
(1,372)	1:38:A:LEU:HA	1:41:A:LEU:HD23	3	0.35	0.13	0.4
(1,502)	1:51:A:LEU:HD22	1:55:A:VAL:HG12	3	0.33	0.07	0.35
(1,502)	1:51:A:LEU:HD23	1:55:A:VAL:HG12	3	0.33	0.07	0.35
(1,502)	1:51:A:LEU:HD11	1:55:A:VAL:HG13	3	0.33	0.07	0.35
(1,502)	1:51:A:LEU:HD12	1:55:A:VAL:HG13	3	0.33	0.07	0.35
(1,502)	1:51:A:LEU:HD13	1:55:A:VAL:HG13	3	0.33	0.07	0.35
(1,1076)	1:105:A:LEU:HD21	1:106:A:LYS:H	3	0.32	0.13	0.4
(1,644)	1:60:A:GLU:H	1:61:A:LEU:HD22	3	0.29	0.15	0.25
(1,644)	1:60:A:GLU:H	1:61:A:LEU:HD23	3	0.29	0.15	0.25
(1,959)	1:97:A:ARG:HG3	1:101:A:GLU:H	3	0.28	0.07	0.3
(1,959)	1:97:A:ARG:HG2	1:101:A:GLU:H	3	0.28	0.07	0.3
(1,80)	1:20:A:LEU:H	1:22:A:PHE:H	3	0.27	0.17	0.19
(1,480)	1:51:A:LEU:HD21	1:52:A:GLY:H	3	0.27	0.06	0.3
(1,38)	1:17:A:GLN:HA	1:21:A:ARG:H	3	0.24	0.06	0.21
(1,897)	1:94:A:VAL:HA	1:95:A:GLU:H	3	0.23	0.07	0.22
(1,99)	1:21:A:ARG:HA	1:22:A:PHE:H	3	0.2	0.04	0.19
(1,623)	1:59:A:GLU:HA	1:104:A:LEU:HD22	3	0.19	0.07	0.18
(1,623)	1:59:A:GLU:HA	1:104:A:LEU:HD23	3	0.19	0.07	0.18
(1,447)	1:48:A:ARG:HA	1:49:A:GLU:H	3	0.18	0.05	0.15
(1,206)	1:27:A:LYS:HA	1:28:A:ASN:H	3	0.15	0.03	0.14
(1,78)	1:20:A:LEU:HA	1:21:A:ARG:H	3	0.15	0.03	0.13
(1,596)	1:58:A:VAL:HG11	1:96:A:LEU:HD21	3	0.14	0.03	0.13
(1,475)	1:51:A:LEU:HA	1:52:A:GLY:H	3	0.14	0.01	0.14
(1,439)	1:47:A:GLU:HA	1:48:A:ARG:H	3	0.13	0.01	0.13
(1,867)	1:90:A:LYS:HA	1:91:A:ALA:H	3	0.13	0.02	0.13
(1,1055)	1:104:A:LEU:HA	1:105:A:LEU:H	3	0.12	0.03	0.11
(1,636)	1:60:A:GLU:HA	1:61:A:LEU:H	3	0.12	0.03	0.1
(1,755)	1:71:A:LEU:HD21	1:74:A:GLU:HG2	2	0.79	0.5	0.79
(1,592)	1:58:A:VAL:HG23	1:61:A:LEU:HD21	2	0.78	0.01	0.78
(1,505)	1:51:A:LEU:HD21	1:55:A:VAL:HG21	2	0.68	0.3	0.68

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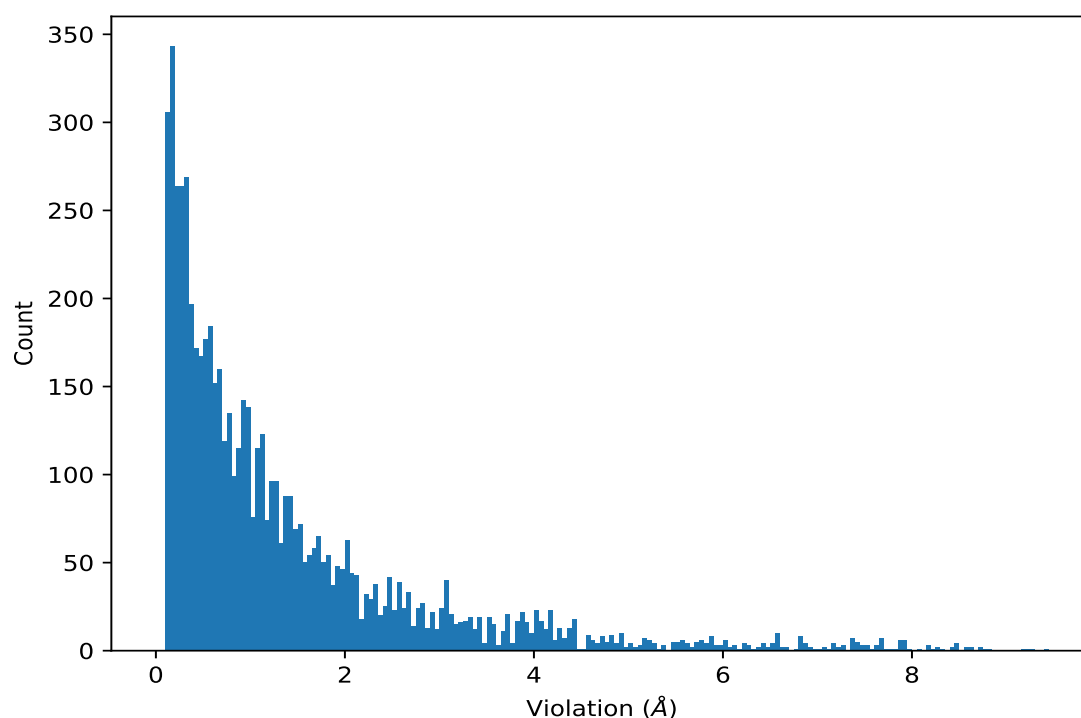
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,939)	1:96:A:LEU:HD13	1:100:A:LEU:HD21	2	0.6	0.34	0.6
(1,270)	1:32:A:ASN:HB3	1:34:A:LEU:HD21	2	0.58	0.29	0.58
(1,148)	1:23:A:VAL:HG22	1:26:A:LEU:HD21	2	0.44	0.2	0.44
(1,1052)	1:103:A:VAL:HA	1:106:A:LYS:H	2	0.4	0.0	0.4
(1,282)	1:33:A:ASP:HA	1:36:A:LEU:HD11	2	0.35	0.17	0.35
(1,282)	1:33:A:ASP:HA	1:36:A:LEU:HD12	2	0.35	0.17	0.35
(1,282)	1:33:A:ASP:HA	1:36:A:LEU:HD13	2	0.35	0.17	0.35
(1,199)	1:26:A:LEU:HD21	1:29:A:ALA:HB3	2	0.34	0.06	0.34
(1,468)	1:50:A:ALA:HA	1:53:A:THR:H	2	0.26	0.04	0.26
(1,166)	1:25:A:LEU:H	1:26:A:LEU:H	2	0.24	0.05	0.24
(1,638)	1:60:A:GLU:HA	1:63:A:ARG:H	2	0.24	0.04	0.24
(1,607)	1:58:A:VAL:HG23	1:96:A:LEU:HD22	2	0.24	0.08	0.24
(1,607)	1:58:A:VAL:HG23	1:96:A:LEU:HD23	2	0.24	0.08	0.24
(1,1066)	1:104:A:LEU:H	1:106:A:LYS:H	2	0.21	0.11	0.21
(1,691)	1:64:A:GLY:H	1:66:A:MET:H	2	0.2	0.08	0.2
(1,757)	1:72:A:LYS:HA	1:73:A:ASN:H	2	0.2	0.04	0.2
(1,431)	1:46:A:ASP:HA	1:47:A:GLU:H	2	0.19	0.05	0.19
(1,909)	1:95:A:GLU:HA	1:96:A:LEU:H	2	0.18	0.02	0.18
(1,297)	1:35:A:HIS:HE1	1:36:A:LEU:H	2	0.16	0.02	0.16
(1,443)	1:47:A:GLU:HA	1:50:A:ALA:H	2	0.16	0.02	0.16
(1,875)	1:91:A:ALA:HA	1:92:A:ALA:H	2	0.16	0.06	0.16
(1,856)	1:89:A:LEU:HD11	1:92:A:ALA:H	2	0.16	0.04	0.16
(1,856)	1:89:A:LEU:HD12	1:92:A:ALA:H	2	0.16	0.04	0.16
(1,856)	1:89:A:LEU:HD13	1:92:A:ALA:H	2	0.16	0.04	0.16
(1,650)	1:61:A:LEU:HA	1:64:A:GLY:H	2	0.16	0.04	0.16
(1,336)	1:36:A:LEU:H	1:37:A:PRO:HG3	2	0.14	0.02	0.14
(1,336)	1:36:A:LEU:H	1:37:A:PRO:HG2	2	0.14	0.02	0.14
(1,406)	1:42:A:MET:HA	1:43:A:LEU:H	2	0.14	0.03	0.14
(1,21)	1:16:A:HIS:HA	1:18:A:GLU:H	2	0.14	0.01	0.14
(1,962)	1:98:A:GLN:HA	1:99:A:TRP:H	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	13	9.44
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	3	9.28
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	12	9.21
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	13	9.16
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	2	8.83
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	6	8.77
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	11	8.74
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	14	8.72
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	9	8.62
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	1	8.6
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	7	8.59
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	3	8.55
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	9	8.48
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	5	8.47
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	14	8.46
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	8	8.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	12	8.43
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	3	8.4
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	2	8.33
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	13	8.29
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	8	8.26
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	3	8.2
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	1	8.19
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	2	8.19
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	12	8.16
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	6	8.07
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	7	7.98
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	1	7.94
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	1	7.94
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	13	7.93
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	13	7.93
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	3	7.92
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	11	7.91
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	14	7.89
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	14	7.89
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	10	7.89
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	12	7.86
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	12	7.86
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	12	7.86
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	15	7.82
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	1	7.79
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	14	7.71
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	3	7.69
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	3	7.69
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	2	7.67
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	2	7.67
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	1	7.67
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	1	7.67
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	5	7.67
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	11	7.6
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	4	7.6
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	6	7.6
(1,661)	1:61:A:LEU:HD21	1:96:A:LEU:HD13	10	7.58
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	5	7.54
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	2	7.52
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	6	7.52
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	2	7.47
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	13	7.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	15	7.45
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	4	7.43
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	4	7.43
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	9	7.43
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	4	7.41
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	1	7.4
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	6	7.37
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	6	7.37
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	8	7.37
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	11	7.37
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	7	7.35
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	11	7.35
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	11	7.35
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	7	7.29
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	5	7.26
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	14	7.26
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	5	7.23
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	1	7.2
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	15	7.19
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	15	7.19
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	12	7.18
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	12	7.18
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	10	7.1
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	4	7.06
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	6	7.05
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	12	7.0
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	12	6.98
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	3	6.92
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	12	6.91
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	3	6.88
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	7	6.87
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	7	6.87
(1,659)	1:61:A:LEU:HD21	1:96:A:LEU:HD12	4	6.85
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	9	6.84
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	4	6.82
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	4	6.82
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	10	6.82
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	10	6.82
(1,657)	1:61:A:LEU:HD21	1:96:A:LEU:HD11	15	6.82
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	5	6.81
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	5	6.81
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	7	6.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	14	6.69
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	14	6.69
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	12	6.61
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	12	6.61
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	8	6.59
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	8	6.59
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	2	6.59
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	2	6.59
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	6	6.59
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	6	6.59
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	11	6.57
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	11	6.57
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	3	6.55
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	3	6.55
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	1	6.51
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	1	6.51
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	13	6.5
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	13	6.5
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	5	6.45
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	5	6.45
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	11	6.43
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	11	6.43
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	11	6.43
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	13	6.42
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	7	6.39
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	8	6.37
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	15	6.34
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	4	6.29
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	6	6.28
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	8	6.25
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	10	6.24
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	9	6.23
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	9	6.23
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	11	6.21
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	7	6.17
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	14	6.14
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	12	6.1
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	2	6.1
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	2	6.06
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	11	6.05
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	6	6.04
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	13	6.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	12	6.03
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	11	6.02
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	9	6.0
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	9	6.0
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	9	5.98
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	15	5.96
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	15	5.96
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	13	5.94
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	6	5.93
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	3	5.93
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	2	5.89
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	10	5.88
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	10	5.88
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	5	5.88
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	14	5.88
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	8	5.87
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	8	5.87
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	12	5.86
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	9	5.82
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	12	5.81
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	12	5.81
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	9	5.8
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	1	5.79
(1,662)	1:61:A:LEU:HD22	1:96:A:LEU:HD13	7	5.78
(1,662)	1:61:A:LEU:HD23	1:96:A:LEU:HD13	7	5.78
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	11	5.78
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	10	5.76
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	10	5.76
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	7	5.74
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	14	5.73
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	14	5.72
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	14	5.72
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	14	5.72
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	14	5.68
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	12	5.68
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	7	5.64
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	1	5.64
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	14	5.61
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	14	5.61
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	15	5.59
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	15	5.59
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	15	5.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	5	5.58
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	9	5.58
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	1	5.57
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	10	5.54
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	15	5.54
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	7	5.53
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	10	5.52
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	10	5.51
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	4	5.48
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	13	5.47
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	13	5.47
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	15	5.46
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	15	5.46
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	14	5.38
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	8	5.38
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	9	5.37
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	14	5.31
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	12	5.29
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	11	5.27
(1,766)	1:75:A:LEU:H	1:79:A:ILE:HB	13	5.25
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	5	5.25
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	15	5.24
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	10	5.23
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	15	5.22
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	15	5.22
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	13	5.21
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	11	5.2
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	8	5.18
(1,783)	1:76:A:GLY:H	1:79:A:ILE:HB	13	5.16
(1,770)	1:76:A:GLY:H	1:79:A:ILE:HB	13	5.16
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	1	5.16
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	1	5.16
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	4	5.15
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	3	5.15
(1,257)	1:31:A:GLN:HG2	1:34:A:LEU:HD21	6	5.14
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	11	5.14
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	13	5.12
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	10	5.09
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	13	5.08
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	14	5.04
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	7	5.04
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	2	5.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	15	5.02
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	11	4.99
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	11	4.99
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	13	4.94
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	6	4.93
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	6	4.93
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	3	4.93
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	3	4.93
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	14	4.91
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	8	4.91
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	13	4.9
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	13	4.9
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	13	4.9
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	8	4.89
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	6	4.89
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	6	4.88
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	6	4.88
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	8	4.84
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	1	4.81
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	1	4.81
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	1	4.81
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	1	4.81
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	14	4.8
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	14	4.8
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	5	4.8
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	5	4.8
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	9	4.79
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	9	4.79
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	1	4.78
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	3	4.76
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	3	4.76
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	3	4.72
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	1	4.7
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	1	4.7
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	5	4.7
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	5	4.7
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	11	4.7
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	5	4.7
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	13	4.7
(1,664)	1:61:A:LEU:HD21	1:96:A:LEU:HD21	4	4.68
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	1	4.68
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	8	4.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	4	4.65
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	10	4.64
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	10	4.64
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	15	4.63
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	15	4.63
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	1	4.62
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	10	4.6
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	10	4.59
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	10	4.59
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	9	4.57
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	10	4.57
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	9	4.55
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	9	4.55
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	7	4.55
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	7	4.55
(1,255)	1:31:A:GLN:HG3	1:34:A:LEU:HD21	6	4.55
(1,667)	1:61:A:LEU:HD21	1:96:A:LEU:HD22	15	4.51
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	6	4.48
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	5	4.44
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	10	4.43
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	13	4.43
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	13	4.43
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	13	4.43
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	13	4.43
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	13	4.43
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	6	4.43
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	6	4.43
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	6	4.43
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	13	4.42
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	4	4.42
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	4	4.42
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	7	4.41
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	15	4.41
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	7	4.41
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	7	4.41
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	12	4.4
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	13	4.38
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	13	4.38
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	13	4.38
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	13	4.38
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	13	4.38
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	14	4.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	14	4.38
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	14	4.38
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	14	4.38
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	14	4.38
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	1	4.36
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	6	4.36
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	6	4.36
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	2	4.34
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	2	4.34
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	2	4.34
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	2	4.34
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	10	4.34
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	2	4.31
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	2	4.31
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	12	4.29
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	12	4.29
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	12	4.29
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	14	4.29
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	14	4.29
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	14	4.29
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	9	4.28
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	4	4.28
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	4	4.27
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	4	4.27
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	9	4.26
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	9	4.25
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	9	4.25
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	8	4.24
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	2	4.24
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	2	4.24
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	2	4.24
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	3	4.23
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	3	4.23
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	2	4.19
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	12	4.19
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	1	4.19
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	1	4.19
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	1	4.19
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	5	4.18
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	5	4.18
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	3	4.18
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	3	4.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	3	4.18
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	1	4.18
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	12	4.17
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	12	4.17
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	14	4.16
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	14	4.16
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	14	4.16
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	14	4.16
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	14	4.16
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	5	4.15
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	10	4.15
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	10	4.15
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	10	4.15
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	10	4.15
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	14	4.14
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	14	4.14
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	8	4.13
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	8	4.13
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	4	4.13
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	4	4.13
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	11	4.12
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	11	4.12
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	11	4.1
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	13	4.1
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	13	4.1
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	13	4.1
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	7	4.09
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	7	4.09
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	2	4.08
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	2	4.08
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	2	4.08
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	2	4.08
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	2	4.08
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	2	4.08
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	3	4.07
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	11	4.07
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	11	4.07
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	2	4.06
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	2	4.06
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	6	4.06
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	15	4.06
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	15	4.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	2	4.05
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	10	4.04
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	10	4.04
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	10	4.04
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	1	4.03
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	1	4.03
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	1	4.03
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	1	4.03
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	1	4.03
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	1	4.03
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	14	4.02
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	14	4.02
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	14	4.02
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	3	4.02
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	3	4.02
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	3	4.02
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	3	4.0
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	3	4.0
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	3	4.0
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	3	4.0
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	2	4.0
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	15	4.0
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	15	4.0
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	15	4.0
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	13	3.99
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	13	3.99
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	4	3.99
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	4	3.99
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	4	3.99
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	4	3.99
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	5	3.99
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	5	3.99
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	5	3.99
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	3	3.96
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	12	3.93
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	12	3.93
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	5	3.93
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	6	3.92
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	6	3.92
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	6	3.92
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	6	3.92
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	7	3.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	7	3.91
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	7	3.91
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	7	3.91
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	11	3.91
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	11	3.91
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	11	3.91
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	1	3.91
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	9	3.9
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	9	3.89
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	9	3.89
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	12	3.89
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	12	3.89
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	12	3.89
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	12	3.89
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	12	3.89
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	11	3.89
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	11	3.89
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	14	3.87
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	7	3.87
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	7	3.87
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	6	3.87
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	6	3.87
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	6	3.87
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	1	3.86
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	1	3.86
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	1	3.86
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	1	3.86
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	1	3.86
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	14	3.85
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	14	3.85
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	4	3.84
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	4	3.84
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	4	3.84
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	4	3.84
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	4	3.84
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	4	3.84
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	9	3.84
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	2	3.83
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	2	3.83
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	2	3.83
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	2	3.81
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	2	3.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	3	3.81
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	3	3.81
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	8	3.8
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	8	3.8
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	5	3.8
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	14	3.79
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	14	3.79
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	14	3.79
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	9	3.78
(1,887)	1:92:A:ALA:HA	1:95:A:GLU:H	4	3.74
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	6	3.74
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	6	3.74
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	13	3.74
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	13	3.74
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	13	3.74
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	13	3.74
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	6	3.73
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	10	3.72
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	3	3.71
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	3	3.71
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	3	3.71
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	3	3.71
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	3	3.71
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	3	3.71
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	12	3.71
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	12	3.71
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	12	3.71
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	1	3.7
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	1	3.7
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	14	3.7
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	4	3.69
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	4	3.69
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	4	3.69
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	2	3.69
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	6	3.68
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB3	7	3.67
(1,841)	1:88:A:SER:HA	1:93:A:PRO:HB2	7	3.67
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	5	3.67
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	5	3.67
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	5	3.67
(1,669)	1:61:A:LEU:HD21	1:96:A:LEU:HD23	4	3.66
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	9	3.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	9	3.61
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	9	3.61
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	4	3.59
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	5	3.57
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	11	3.57
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	11	3.57
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	11	3.57
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	11	3.57
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	11	3.57
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	15	3.57
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	15	3.57
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	15	3.57
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	15	3.57
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	15	3.57
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	12	3.57
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	12	3.57
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	12	3.57
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	8	3.54
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	8	3.54
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	8	3.54
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	5	3.53
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	15	3.53
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	9	3.53
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	9	3.53
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	9	3.53
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	7	3.53
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	4	3.52
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	10	3.52
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	10	3.52
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	5	3.51
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	5	3.51
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	5	3.51
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	5	3.51
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	5	3.51
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	5	3.51
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	12	3.5
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	15	3.49
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	11	3.47
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	5	3.45
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	4	3.45
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	13	3.44
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	6	3.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	6	3.44
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	7	3.43
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	13	3.43
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	13	3.43
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	13	3.43
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	8	3.43
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	8	3.43
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	9	3.41
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	6	3.41
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	6	3.41
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	6	3.41
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	6	3.41
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	6	3.41
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	4	3.41
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	3	3.4
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	8	3.4
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	13	3.4
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	5	3.39
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	13	3.39
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD11	7	3.38
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD12	7	3.38
(1,651)	1:61:A:LEU:HB3	1:96:A:LEU:HD13	7	3.38
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	1	3.36
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	1	3.36
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	1	3.36
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	1	3.36
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	1	3.36
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	4	3.35
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	4	3.35
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	11	3.34
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	1	3.33
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	1	3.33
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	12	3.33
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	12	3.33
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	8	3.33
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	1	3.32
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	1	3.32
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	1	3.32
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	3	3.32
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	2	3.31
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	10	3.3
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	10	3.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	10	3.3
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	10	3.3
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	10	3.3
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	3	3.3
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	3	3.3
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	11	3.3
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	7	3.29
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	6	3.29
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	6	3.29
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	6	3.29
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	14	3.29
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	15	3.28
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	15	3.28
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	15	3.28
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	15	3.28
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	15	3.28
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	3	3.27
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	10	3.26
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	6	3.26
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	5	3.25
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	3	3.25
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	7	3.25
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	9	3.25
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	12	3.24
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	6	3.23
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	12	3.22
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	3	3.22
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	3	3.22
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	3	3.22
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	3	3.22
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	3	3.22
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	6	3.22
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	12	3.21
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	12	3.21
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	15	3.21
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	10	3.2
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	3	3.2
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	3	3.2
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	3	3.2
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	11	3.19
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	7	3.19
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	7	3.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	7	3.19
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	7	3.19
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	12	3.18
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	12	3.18
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	12	3.18
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	12	3.18
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	12	3.18
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	2	3.18
(1,652)	1:61:A:LEU:HB3	1:96:A:LEU:HD21	8	3.17
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	8	3.16
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	10	3.16
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	13	3.15
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	12	3.14
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	15	3.14
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	1	3.14
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	11	3.14
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	2	3.14
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	5	3.13
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	5	3.13
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	5	3.13
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	5	3.13
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	1	3.13
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	4	3.12
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	8	3.12
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	8	3.12
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	8	3.12
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	8	3.11
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	6	3.11
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	6	3.11
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	6	3.11
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	6	3.11
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	6	3.11
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	12	3.1
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	2	3.09
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	9	3.09
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	2	3.09
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	2	3.09
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	2	3.09
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	2	3.09
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	2	3.09
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	9	3.08
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	13	3.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:61:A:LEU:HD22	1:96:A:LEU:HD21	8	3.08
(1,665)	1:61:A:LEU:HD23	1:96:A:LEU:HD21	8	3.08
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	4	3.08
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	4	3.08
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	4	3.08
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	4	3.08
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	4	3.08
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD22	5	3.08
(1,258)	1:31:A:GLN:HG2	1:34:A:LEU:HD23	5	3.08
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	11	3.07
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	11	3.07
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	11	3.07
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	9	3.07
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	9	3.07
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	9	3.07
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	9	3.07
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	9	3.07
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	11	3.07
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	11	3.07
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	11	3.07
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	11	3.07
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	11	3.07
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	15	3.07
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	15	3.07
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	15	3.07
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	1	3.07
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	1	3.07
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	1	3.07
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	1	3.07
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	1	3.07
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	4	3.05
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	14	3.04
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	10	3.04
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	10	3.04
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	5	3.02
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	5	3.02
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	5	3.02
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	5	3.02
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	5	3.02
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	2	3.02
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	3	3.02
(1,175)	1:25:A:LEU:HD21	1:28:A:ASN:HA	3	3.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	7	3.01
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	7	3.01
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	7	3.01
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	7	3.01
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	7	3.01
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	7	3.01
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	8	3.01
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	4	3.01
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	4	3.01
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	4	3.01
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	8	3.01
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	1	3.01
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	6	3.0
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	5	2.99
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	2	2.99
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	9	2.98
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	12	2.98
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	1	2.98
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	11	2.97
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	15	2.97
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	15	2.96
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	4	2.95
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	4	2.95
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	4	2.95
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	7	2.95
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	7	2.94
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	10	2.94
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	10	2.94
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	10	2.94
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	10	2.94
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	10	2.94
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	4	2.94
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	1	2.94
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	11	2.93
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	13	2.93
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	11	2.93
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	11	2.93
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	11	2.93
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	7	2.93
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	1	2.93
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	14	2.92
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	9	2.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	13	2.91
(1,602)	1:58:A:VAL:HG21	1:96:A:LEU:HD21	14	2.91
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	15	2.9
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	15	2.9
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	15	2.9
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	11	2.88
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	7	2.88
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	7	2.88
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	7	2.88
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	7	2.88
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	7	2.88
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	3	2.88
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	13	2.88
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	10	2.87
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	14	2.87
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	4	2.86
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	6	2.86
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	5	2.85
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	14	2.84
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	3	2.84
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	3	2.84
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	3	2.84
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	3	2.84
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	3	2.84
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	2	2.84
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	2	2.84
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	5	2.83
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	15	2.83
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	5	2.82
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	5	2.82
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	5	2.82
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	9	2.82
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	9	2.82
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	2	2.81
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	2	2.81
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	2	2.81
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	2	2.81
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	2	2.81
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	11	2.81
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	5	2.81
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	3	2.8
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	3	2.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	1	2.8
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	1	2.8
(1,346)	1:37:A:PRO:HA	1:38:A:LEU:HD21	12	2.8
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	5	2.79
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	6	2.78
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	6	2.78
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	6	2.78
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	6	2.78
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	6	2.78
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	6	2.78
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	7	2.78
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	7	2.78
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	7	2.78
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	5	2.78
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	5	2.78
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	10	2.78
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	6	2.76
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	12	2.75
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	4	2.75
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	4	2.75
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	14	2.75
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	14	2.75
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	14	2.75
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	2	2.75
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	2	2.75
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	2	2.75
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	15	2.75
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	2	2.74
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	5	2.73
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	5	2.73
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	5	2.73
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	11	2.72
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	11	2.72
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	6	2.71
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	6	2.71
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	14	2.71
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	5	2.71
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	9	2.7
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	13	2.7
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	5	2.7
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	5	2.7
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	5	2.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	5	2.69
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	5	2.69
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	5	2.69
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	5	2.69
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	14	2.69
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	14	2.69
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	14	2.69
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	11	2.68
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	11	2.68
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	11	2.68
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	11	2.68
(1,767)	1:75:A:LEU:HA	1:78:A:GLY:H	10	2.68
(1,660)	1:61:A:LEU:HD22	1:96:A:LEU:HD12	8	2.68
(1,660)	1:61:A:LEU:HD23	1:96:A:LEU:HD12	8	2.68
(1,660)	1:61:A:LEU:HD11	1:96:A:LEU:HD13	8	2.68
(1,660)	1:61:A:LEU:HD12	1:96:A:LEU:HD13	8	2.68
(1,660)	1:61:A:LEU:HD13	1:96:A:LEU:HD13	8	2.68
(1,670)	1:61:A:LEU:HD22	1:96:A:LEU:HD23	8	2.67
(1,670)	1:61:A:LEU:HD23	1:96:A:LEU:HD23	8	2.67
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	3	2.66
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	1	2.66
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	1	2.66
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	1	2.66
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	1	2.66
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	1	2.66
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	12	2.66
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	4	2.66
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	3	2.65
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	3	2.65
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	5	2.65
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	5	2.65
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	10	2.65
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	8	2.64
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	8	2.64
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	6	2.64
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	6	2.64
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	7	2.63
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	7	2.63
(1,654)	1:61:A:LEU:HB2	1:96:A:LEU:HD21	8	2.63
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	4	2.62
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	4	2.62
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	14	2.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	14	2.62
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	14	2.62
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	10	2.62
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	10	2.62
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	10	2.62
(1,606)	1:58:A:VAL:HG23	1:96:A:LEU:HD21	15	2.62
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	6	2.61
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	3	2.61
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	15	2.6
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	4	2.6
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	13	2.6
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	9	2.6
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	9	2.6
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	9	2.6
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	15	2.59
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	15	2.59
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	8	2.59
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	1	2.59
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	2	2.59
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	12	2.58
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	12	2.58
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	12	2.58
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	13	2.58
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	7	2.58
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	7	2.58
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	12	2.58
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	12	2.58
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	14	2.58
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	14	2.58
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	15	2.57
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	15	2.57
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	11	2.57
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	13	2.57
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	13	2.57
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	2	2.56
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	2	2.56
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	12	2.56
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	12	2.56
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	12	2.56
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	12	2.56
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	12	2.56
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	14	2.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	11	2.55
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	11	2.55
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	13	2.55
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	13	2.55
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	8	2.55
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	11	2.55
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	11	2.55
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	10	2.55
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	10	2.55
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	10	2.55
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	10	2.55
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	1	2.54
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	1	2.54
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	1	2.54
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	1	2.54
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	1	2.54
(1,358)	1:37:A:PRO:HB2	1:41:A:LEU:HD21	15	2.54
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	7	2.53
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	7	2.53
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	7	2.53
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	7	2.53
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	7	2.53
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	10	2.53
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	10	2.53
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	8	2.53
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	15	2.52
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	14	2.52
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	3	2.51
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	3	2.51
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	7	2.51
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	6	2.51
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	4	2.5
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	4	2.5
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	4	2.5
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	6	2.49
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	6	2.49
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	13	2.49
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	13	2.49
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	13	2.49
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	13	2.49
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	13	2.49
(1,602)	1:58:A:VAL:HG21	1:96:A:LEU:HD21	9	2.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	13	2.49
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	13	2.49
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	13	2.49
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	10	2.49
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	14	2.49
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	7	2.48
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	7	2.48
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	7	2.48
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	7	2.48
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	4	2.48
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	4	2.48
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	15	2.48
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	15	2.48
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	4	2.47
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	4	2.47
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	4	2.47
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	4	2.47
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	4	2.47
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	15	2.47
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	9	2.47
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	15	2.46
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	15	2.46
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	1	2.46
(1,656)	1:61:A:LEU:HD11	1:96:A:LEU:HD11	2	2.46
(1,656)	1:61:A:LEU:HD12	1:96:A:LEU:HD11	2	2.46
(1,656)	1:61:A:LEU:HD13	1:96:A:LEU:HD11	2	2.46
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	4	2.46
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	6	2.45
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	12	2.45
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	12	2.45
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	1	2.45
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	1	2.45
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	3	2.45
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	11	2.45
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	11	2.44
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	3	2.44
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	3	2.44
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	9	2.44
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	9	2.44
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	9	2.44
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	9	2.44
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	9	2.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	9	2.44
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	9	2.44
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	10	2.43
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	10	2.43
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	12	2.43
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	12	2.43
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	13	2.43
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	13	2.43
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	3	2.43
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	5	2.43
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	15	2.42
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	15	2.42
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	15	2.42
(1,356)	1:37:A:PRO:HB3	1:41:A:LEU:HD21	15	2.42
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	3	2.42
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	7	2.42
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	7	2.4
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	9	2.39
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	9	2.39
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	8	2.39
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	3	2.38
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	3	2.38
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	3	2.38
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	3	2.38
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	3	2.38
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	12	2.38
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	6	2.38
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	15	2.36
(1,602)	1:58:A:VAL:HG21	1:96:A:LEU:HD21	10	2.36
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	6	2.35
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	6	2.35
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	8	2.35
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	8	2.35
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	8	2.35
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	8	2.35
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	8	2.35
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	8	2.35
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	12	2.34
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	12	2.34
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	12	2.34
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	12	2.34
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	13	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	13	2.34
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	13	2.34
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	3	2.34
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	3	2.34
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	3	2.34
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	6	2.33
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	9	2.33
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	4	2.33
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	4	2.33
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	8	2.33
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	9	2.32
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	9	2.32
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	6	2.32
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	6	2.32
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	13	2.32
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	13	2.32
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	11	2.31
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	11	2.31
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	14	2.31
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	14	2.31
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	14	2.31
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	14	2.31
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	14	2.31
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	14	2.31
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	14	2.31
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	2	2.31
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	2	2.31
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	9	2.31
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	14	2.31
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	15	2.3
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	15	2.3
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	2	2.3
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	7	2.3
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	2	2.29
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	2	2.29
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	2	2.29
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	2	2.29
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	2	2.29
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	7	2.29
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	8	2.28
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	8	2.28
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	4	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	4	2.27
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	11	2.27
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	11	2.27
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	8	2.26
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	8	2.26
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	8	2.26
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	8	2.26
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	8	2.26
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	8	2.26
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	4	2.26
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	6	2.26
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	14	2.25
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	14	2.25
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	9	2.25
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	9	2.25
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	9	2.25
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	15	2.25
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	15	2.25
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	15	2.25
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	7	2.25
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	15	2.24
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	8	2.24
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	8	2.24
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	8	2.24
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	9	2.24
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	9	2.24
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	7	2.24
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	14	2.24
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	11	2.23
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	11	2.23
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	14	2.23
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	14	2.23
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	14	2.23
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	14	2.23
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	14	2.23
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	8	2.23
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	10	2.23
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	10	2.23
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	10	2.23
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	6	2.23
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	5	2.22
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	12	2.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	1	2.22
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	10	2.22
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	5	2.21
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	12	2.21
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	12	2.21
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	12	2.21
(1,176)	1:25:A:LEU:HD22	1:28:A:ASN:HA	3	2.21
(1,176)	1:25:A:LEU:HD23	1:28:A:ASN:HA	3	2.21
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	11	2.2
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	14	2.2
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	12	2.19
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	6	2.19
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	6	2.19
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	6	2.19
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	3	2.19
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	5	2.17
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	5	2.17
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	4	2.16
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	9	2.16
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	12	2.16
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	12	2.16
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	12	2.16
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	12	2.16
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	12	2.16
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	7	2.16
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	7	2.16
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	7	2.16
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	14	2.15
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	14	2.14
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	14	2.14
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	2	2.14
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	9	2.14
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	9	2.14
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	9	2.14
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	12	2.14
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	13	2.14
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	2	2.13
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	2	2.13
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	2	2.13
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	2	2.13
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	2	2.13
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	2	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	2	2.13
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	2	2.13
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	2	2.13
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	8	2.13
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	8	2.13
(1,349)	1:37:A:PRO:HG3	1:38:A:LEU:HD21	6	2.13
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	11	2.13
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	11	2.12
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	11	2.12
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	11	2.12
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	11	2.12
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	11	2.12
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	11	2.12
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	7	2.12
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	7	2.12
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	7	2.12
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	12	2.12
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	9	2.11
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	11	2.11
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	11	2.11
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	13	2.11
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	13	2.11
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	13	2.11
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	13	2.11
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	13	2.11
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	5	2.11
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	11	2.11
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	6	2.1
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	5	2.1
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	12	2.09
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	8	2.08
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	9	2.08
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	9	2.08
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	9	2.08
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	9	2.08
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	3	2.08
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	3	2.08
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	10	2.08
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	10	2.08
(1,606)	1:58:A:VAL:HG23	1:96:A:LEU:HD21	14	2.08
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	14	2.08
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	12	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	15	2.08
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	15	2.08
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	15	2.08
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	10	2.08
(1,658)	1:61:A:LEU:HD22	1:96:A:LEU:HD11	8	2.07
(1,658)	1:61:A:LEU:HD23	1:96:A:LEU:HD11	8	2.07
(1,658)	1:61:A:LEU:HD11	1:96:A:LEU:HD12	8	2.07
(1,658)	1:61:A:LEU:HD12	1:96:A:LEU:HD12	8	2.07
(1,658)	1:61:A:LEU:HD13	1:96:A:LEU:HD12	8	2.07
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	1	2.07
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	1	2.07
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	9	2.07
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	10	2.06
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	10	2.06
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	10	2.06
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	10	2.06
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	10	2.06
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	15	2.06
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	8	2.05
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	1	2.05
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	1	2.05
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	1	2.05
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	1	2.05
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	1	2.05
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	1	2.05
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	1	2.05
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	1	2.05
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	1	2.05
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	5	2.05
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	5	2.05
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	5	2.05
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	1	2.04
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	1	2.04
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	1	2.04
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	5	2.04
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	5	2.04
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	5	2.04
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	11	2.03
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	15	2.03
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	5	2.03
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	5	2.03
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	10	2.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	10	2.03
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	14	2.03
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	14	2.03
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	2	2.03
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	11	2.03
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	11	2.03
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	11	2.03
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	6	2.03
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	6	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	6	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	6	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	6	2.03
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	11	2.03
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	11	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	11	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	11	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	11	2.03
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	15	2.03
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	15	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	15	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	15	2.03
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	15	2.03
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	1	2.03
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	1	2.03
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	1	2.03
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	2	2.03
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	12	2.03
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	12	2.03
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	12	2.03
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	9	2.03
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	9	2.03
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	9	2.03
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	13	2.02
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	7	2.02
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	13	2.01
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	7	2.01
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	7	2.01
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	7	2.01
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	7	2.01
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	7	2.01
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	8	2.01
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	12	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	3	2.0
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	3	2.0
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	3	2.0
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	3	2.0
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	3	2.0
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	6	2.0
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	6	2.0
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	6	2.0
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	7	2.0
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	12	2.0
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	10	1.99
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	10	1.99
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	10	1.99
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	5	1.99
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	5	1.99
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	5	1.99
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	5	1.99
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	5	1.99
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	15	1.99
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	15	1.99
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	2	1.99
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	7	1.99
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	13	1.98
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	13	1.98
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	2	1.98
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	12	1.98
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	12	1.98
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	12	1.98
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	2	1.97
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	7	1.97
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	7	1.97
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	1	1.97
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	1	1.97
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	1	1.97
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	13	1.97
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	4	1.96
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	10	1.96
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	10	1.96
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	10	1.96
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	10	1.96
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	4	1.96
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	4	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	12	1.96
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	12	1.96
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	1	1.96
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	1	1.96
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	1	1.96
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	7	1.96
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	5	1.95
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	6	1.95
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	5	1.95
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	13	1.95
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	13	1.95
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	15	1.95
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	15	1.95
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	4	1.95
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	1	1.94
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	1	1.94
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	8	1.94
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	8	1.94
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	12	1.94
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	12	1.94
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	1	1.94
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	1	1.94
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	6	1.94
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	4	1.94
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	12	1.93
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	1	1.93
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	1	1.93
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	1	1.93
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	10	1.93
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	8	1.93
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	8	1.93
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	8	1.93
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	8	1.93
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	8	1.93
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	8	1.93
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	7	1.92
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	7	1.92
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	4	1.92
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	13	1.91
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	13	1.91
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	13	1.91
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	12	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	12	1.91
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	2	1.91
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	1	1.91
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	6	1.91
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	13	1.91
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	6	1.91
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	6	1.91
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	6	1.91
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	6	1.91
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	6	1.91
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	9	1.91
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	9	1.91
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	8	1.91
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	10	1.91
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	10	1.91
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	5	1.91
(1,699)	1:65:A:GLU:HA	1:67:A:SER:H	7	1.9
(1,602)	1:58:A:VAL:HG21	1:96:A:LEU:HD21	13	1.9
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	8	1.9
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	13	1.9
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	6	1.89
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	1	1.89
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	1	1.89
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	12	1.89
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	12	1.89
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	4	1.89
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	15	1.89
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	14	1.88
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	14	1.88
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	13	1.88
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	6	1.88
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	6	1.88
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	6	1.88
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	7	1.87
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	7	1.87
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	5	1.87
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	5	1.87
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	1	1.87
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	1	1.87
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	1	1.87
(1,328)	1:36:A:LEU:HD21	1:39:A:LEU:HD21	1	1.87
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	12	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	3	1.86
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	3	1.86
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	3	1.86
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	10	1.86
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	6	1.85
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	14	1.85
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	2	1.85
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	2	1.85
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	2	1.85
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	2	1.85
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	2	1.85
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	13	1.85
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	9	1.85
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	1	1.85
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	13	1.85
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	8	1.84
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	8	1.84
(1,602)	1:58:A:VAL:HG21	1:96:A:LEU:HD21	12	1.84
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	8	1.84
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	8	1.84
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	8	1.84
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	6	1.83
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	4	1.83
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	4	1.83
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	4	1.83
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	2	1.83
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	2	1.83
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	14	1.83
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	14	1.83
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	14	1.83
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	14	1.82
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	14	1.82
(1,646)	1:58:A:VAL:H	1:61:A:LEU:HD21	3	1.82
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	8	1.82
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	8	1.82
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	8	1.82
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	12	1.82
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	12	1.82
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	12	1.82
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	5	1.82
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	5	1.82
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	5	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	7	1.82
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	15	1.82
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	15	1.82
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	2	1.81
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	2	1.81
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	2	1.81
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	7	1.81
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	9	1.81
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	2	1.81
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	2	1.81
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	2	1.81
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	9	1.81
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	9	1.81
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	9	1.81
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	2	1.81
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	13	1.8
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	13	1.8
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	9	1.8
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	9	1.8
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	13	1.8
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	13	1.8
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	5	1.8
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	10	1.8
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	10	1.8
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	8	1.8
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	8	1.8
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	8	1.8
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	7	1.79
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	7	1.79
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	7	1.79
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	13	1.79
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	2	1.78
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	2	1.78
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	2	1.78
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	13	1.78
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	15	1.78
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	8	1.78
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	3	1.78
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	15	1.77
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	15	1.77
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	15	1.77
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	15	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	15	1.77
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	8	1.77
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	3	1.77
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	2	1.76
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	13	1.76
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	6	1.76
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	6	1.76
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	4	1.76
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	4	1.76
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	4	1.76
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	4	1.76
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	4	1.76
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	4	1.76
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	4	1.76
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	4	1.76
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	4	1.76
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	4	1.76
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	3	1.76
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	3	1.76
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	3	1.76
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	8	1.75
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	12	1.75
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	12	1.75
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	12	1.75
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	12	1.75
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	12	1.75
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	12	1.75
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	9	1.75
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	9	1.75
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	12	1.75
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	7	1.75
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	7	1.75
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	7	1.75
(1,602)	1:58:A:VAL:HG21	1:96:A:LEU:HD21	11	1.75
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	13	1.75
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	11	1.74
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	9	1.74
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	2	1.74
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	2	1.74
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	2	1.74
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	13	1.74
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	13	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	13	1.74
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	4	1.74
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	4	1.74
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	14	1.73
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	10	1.73
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	10	1.73
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	3	1.73
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	3	1.73
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	3	1.73
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	3	1.73
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	3	1.73
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	1	1.73
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	1	1.73
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	3	1.73
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	9	1.72
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	14	1.72
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	11	1.72
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	12	1.72
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	12	1.72
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	1	1.72
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	1	1.72
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	1	1.72
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	2	1.72
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	2	1.72
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	2	1.72
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	9	1.72
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	7	1.71
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	7	1.71
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	7	1.71
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	1	1.71
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	4	1.71
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	4	1.71
(1,700)	1:65:A:GLU:HG3	1:67:A:SER:H	2	1.71
(1,700)	1:65:A:GLU:HG2	1:67:A:SER:H	2	1.71
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	12	1.71
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	14	1.71
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	11	1.71
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	6	1.71
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	6	1.71
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	1	1.7
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	2	1.7
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	2	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	2	1.7
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	1	1.7
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	14	1.7
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	14	1.7
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	14	1.7
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	14	1.7
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	7	1.7
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	6	1.7
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	6	1.7
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	4	1.7
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	4	1.7
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	4	1.7
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	6	1.7
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	6	1.7
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	6	1.7
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	1	1.7
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	1	1.69
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	7	1.69
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	11	1.69
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	11	1.69
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	10	1.69
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	3	1.69
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	3	1.69
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	3	1.69
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	7	1.69
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	7	1.69
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	3	1.69
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	3	1.69
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	3	1.69
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	3	1.69
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	3	1.69
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	8	1.69
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	8	1.69
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	8	1.69
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	8	1.69
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	8	1.69
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	1	1.69
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	3	1.69
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	7	1.68
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	3	1.68
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	3	1.68
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	3	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	3	1.68
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	3	1.68
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	3	1.68
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	3	1.68
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	3	1.68
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	3	1.68
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD22	4	1.68
(1,655)	1:61:A:LEU:HB2	1:96:A:LEU:HD23	4	1.68
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	6	1.68
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	12	1.68
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	5	1.67
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	11	1.67
(1,774)	1:76:A:GLY:HA3	1:79:A:ILE:H	10	1.67
(1,774)	1:76:A:GLY:HA2	1:79:A:ILE:H	10	1.67
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	7	1.67
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	2	1.67
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	12	1.67
(1,588)	1:58:A:VAL:HG21	1:61:A:LEU:HD21	6	1.66
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	8	1.65
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	10	1.65
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	6	1.65
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	11	1.65
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	11	1.65
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	10	1.65
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	15	1.65
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	15	1.65
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	15	1.65
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	15	1.65
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	15	1.65
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	11	1.65
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	11	1.65
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	11	1.65
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	2	1.64
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	5	1.64
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	15	1.64
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	15	1.64
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	2	1.64
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	2	1.64
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	2	1.64
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	2	1.64
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	2	1.64
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	4	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	4	1.64
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	4	1.64
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	2	1.64
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	2	1.63
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	8	1.63
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	8	1.63
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	4	1.63
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	4	1.63
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	4	1.63
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	4	1.63
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	4	1.63
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	4	1.63
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	4	1.63
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	4	1.63
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	4	1.63
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	15	1.63
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	15	1.63
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	13	1.63
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	12	1.63
(1,328)	1:36:A:LEU:HD21	1:39:A:LEU:HD21	3	1.63
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	12	1.62
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	10	1.62
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	10	1.62
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	10	1.62
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	10	1.62
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	10	1.62
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	10	1.62
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	5	1.62
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	5	1.62
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	5	1.62
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	13	1.62
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	13	1.62
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	4	1.62
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	4	1.62
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	4	1.62
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	2	1.62
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	5	1.61
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	9	1.61
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	9	1.61
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	9	1.61
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	8	1.6
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	13	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	8	1.6
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	15	1.6
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	2	1.59
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	4	1.59
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	5	1.59
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	5	1.59
(1,606)	1:58:A:VAL:HG23	1:96:A:LEU:HD21	10	1.59
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	4	1.59
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	5	1.59
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	5	1.59
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	6	1.59
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	6	1.59
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	6	1.59
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	4	1.58
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	4	1.58
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	8	1.58
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	8	1.58
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	8	1.58
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	8	1.58
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	8	1.58
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	5	1.57
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	5	1.57
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	5	1.57
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	5	1.57
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	5	1.57
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	5	1.57
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	5	1.57
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	5	1.57
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	5	1.57
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	5	1.57
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	5	1.57
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	5	1.57
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	11	1.57
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	11	1.57
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	11	1.57
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	11	1.57
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	11	1.57
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	11	1.57
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	1	1.56
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	1	1.56
(1,598)	1:58:A:VAL:HG12	1:96:A:LEU:HD21	10	1.56
(1,598)	1:58:A:VAL:HG12	1:96:A:LEU:HD21	14	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	6	1.56
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	6	1.56
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	7	1.56
(1,76)	1:20:A:LEU:HD21	1:21:A:ARG:H	15	1.56
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	13	1.55
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	9	1.55
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	7	1.55
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	14	1.55
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	14	1.55
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	14	1.55
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	7	1.54
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	12	1.54
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	12	1.54
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	10	1.54
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	10	1.54
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	10	1.54
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	1	1.54
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	11	1.54
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	6	1.54
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	11	1.54
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	9	1.54
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	9	1.54
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	9	1.54
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	9	1.54
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	9	1.54
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	7	1.53
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	7	1.53
(1,578)	1:58:A:VAL:HB	1:61:A:LEU:HD21	15	1.53
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	12	1.53
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	12	1.53
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	12	1.53
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	11	1.53
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	14	1.53
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	6	1.53
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	6	1.52
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	8	1.52
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	11	1.52
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	11	1.52
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	5	1.52
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	11	1.52
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	11	1.52
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	11	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	11	1.52
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	11	1.52
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	11	1.52
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	11	1.52
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	11	1.52
(1,598)	1:58:A:VAL:HG12	1:96:A:LEU:HD21	12	1.52
(1,598)	1:58:A:VAL:HG12	1:96:A:LEU:HD21	15	1.52
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	1	1.52
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	1	1.52
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	1	1.52
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	1	1.52
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	1	1.52
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	2	1.52
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	2	1.52
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	2	1.52
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	4	1.52
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	15	1.51
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	15	1.51
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	15	1.51
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	6	1.51
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	6	1.51
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	6	1.51
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	6	1.51
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	6	1.51
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	6	1.51
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	6	1.51
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	6	1.51
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	6	1.51
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	13	1.51
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	3	1.51
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	9	1.51
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	15	1.51
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	12	1.5
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	8	1.5
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	8	1.5
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	8	1.5
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	11	1.5
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	11	1.5
(1,328)	1:36:A:LEU:HD21	1:39:A:LEU:HD21	2	1.5
(1,178)	1:25:A:LEU:HD21	1:28:A:ASN:HB3	11	1.5
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	8	1.49
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	9	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	2	1.49
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	2	1.49
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	14	1.49
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	14	1.49
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	6	1.49
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	3	1.49
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	3	1.49
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	3	1.49
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	12	1.49
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	12	1.49
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	11	1.48
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	11	1.48
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	11	1.48
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	11	1.48
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	8	1.48
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	8	1.48
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	8	1.48
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	8	1.48
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	8	1.48
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	11	1.48
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	13	1.48
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	13	1.48
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	13	1.48
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	1	1.48
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	1	1.48
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	1	1.48
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	1	1.48
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	1	1.48
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	1	1.48
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	7	1.47
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	1	1.47
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	7	1.47
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	7	1.47
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	7	1.47
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	7	1.47
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	7	1.47
(1,606)	1:58:A:VAL:HG23	1:96:A:LEU:HD21	9	1.47
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	11	1.47
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	5	1.47
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	8	1.47
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	6	1.47
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	6	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	6	1.47
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	10	1.46
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	8	1.46
(1,499)	1:51:A:LEU:HD21	1:55:A:VAL:HG11	6	1.46
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	5	1.46
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	14	1.46
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	14	1.46
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	15	1.46
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	10	1.45
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	5	1.45
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	4	1.45
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	4	1.45
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	4	1.45
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	5	1.45
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	6	1.45
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	6	1.45
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	6	1.45
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	14	1.45
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	14	1.45
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	14	1.45
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	14	1.45
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	14	1.45
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	14	1.45
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	14	1.45
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	14	1.45
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	6	1.44
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	7	1.44
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	13	1.44
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	7	1.44
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	7	1.44
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	7	1.44
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	7	1.44
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	7	1.44
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	7	1.44
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	7	1.44
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	7	1.44
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	7	1.44
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	3	1.44
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	3	1.44
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB3	6	1.44
(1,714)	1:67:A:SER:H	1:68:A:GLN:HB2	6	1.44
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	4	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	4	1.44
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	4	1.44
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	3	1.44
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	3	1.44
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	3	1.44
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	3	1.44
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	3	1.44
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	3	1.44
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	11	1.44
(1,942)	1:96:A:LEU:HD21	1:100:A:LEU:HD21	15	1.43
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	13	1.43
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	15	1.43
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	15	1.43
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	15	1.43
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	15	1.43
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	15	1.43
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	15	1.43
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	15	1.43
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	15	1.43
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	15	1.43
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	9	1.43
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	9	1.43
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	9	1.43
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	9	1.43
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	9	1.43
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	8	1.43
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	15	1.43
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	7	1.43
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	8	1.43
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	15	1.43
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	15	1.43
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	15	1.43
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	3	1.43
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	3	1.43
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	3	1.43
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	7	1.42
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	4	1.42
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	12	1.42
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	2	1.42
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	2	1.42
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	5	1.42
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	6	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	6	1.42
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	6	1.42
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	3	1.41
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	1	1.41
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	1	1.41
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	1	1.41
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	6	1.41
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	8	1.41
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	15	1.41
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	15	1.41
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	15	1.41
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	10	1.41
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	10	1.41
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	10	1.41
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	2	1.41
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	10	1.41
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD22	4	1.4
(1,653)	1:61:A:LEU:HB3	1:96:A:LEU:HD23	4	1.4
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD11	4	1.4
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD12	4	1.4
(1,653)	1:61:A:LEU:HB2	1:96:A:LEU:HD13	4	1.4
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	10	1.4
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	14	1.4
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	7	1.4
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	7	1.4
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	7	1.4
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	7	1.4
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	7	1.4
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	13	1.4
(1,1069)	1:104:A:LEU:HD21	1:106:A:LYS:H	10	1.39
(1,974)	1:99:A:TRP:HA	1:103:A:VAL:H	8	1.39
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	6	1.39
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	3	1.39
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	3	1.39
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD22	5	1.39
(1,647)	1:58:A:VAL:H	1:61:A:LEU:HD23	5	1.39
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	4	1.39
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	8	1.39
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	4	1.39
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	1	1.39
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	1	1.39
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	1	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	2	1.39
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	2	1.39
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	2	1.39
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	7	1.39
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	8	1.38
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	15	1.38
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	4	1.38
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	11	1.38
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	11	1.38
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	5	1.38
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	5	1.38
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	5	1.38
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	5	1.38
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	5	1.38
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	9	1.38
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	9	1.38
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	9	1.38
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	11	1.38
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	1	1.37
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	1	1.37
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	5	1.37
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	10	1.37
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	10	1.37
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	10	1.37
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG21	12	1.37
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG21	12	1.37
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG21	12	1.37
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG22	12	1.37
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG22	12	1.37
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG22	12	1.37
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG23	12	1.37
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG23	12	1.37
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG23	12	1.37
(1,292)	1:33:A:ASP:H	1:35:A:HIS:HD2	3	1.37
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	12	1.37
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	9	1.36
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	4	1.36
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	4	1.36
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	7	1.36
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	12	1.36
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	12	1.36
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	12	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	5	1.36
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	5	1.36
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	5	1.36
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	3	1.36
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	2	1.36
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	12	1.36
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	2	1.35
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	9	1.35
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	9	1.35
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	9	1.35
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	1	1.35
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	1	1.35
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	1	1.35
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	2	1.35
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	2	1.35
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	2	1.35
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	11	1.35
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	2	1.35
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	2	1.35
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	2	1.35
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	2	1.35
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	2	1.35
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	2	1.35
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	4	1.35
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	4	1.35
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	4	1.35
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	4	1.35
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	4	1.35
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	4	1.35
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	5	1.35
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	5	1.35
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	5	1.35
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	5	1.35
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	14	1.34
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	7	1.34
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	9	1.34
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	9	1.34
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	9	1.34
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	9	1.34
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	9	1.34
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	9	1.34
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	6	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	12	1.34
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	12	1.34
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	9	1.34
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	5	1.34
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	5	1.34
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	14	1.34
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	1	1.33
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	15	1.33
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	15	1.33
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	15	1.33
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	15	1.33
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	15	1.33
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	15	1.33
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	12	1.33
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	1	1.33
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	5	1.33
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	7	1.33
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	3	1.32
(1,721)	1:67:A:SER:HA	1:71:A:LEU:HD21	2	1.32
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	10	1.32
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	13	1.32
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	13	1.32
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	13	1.32
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	13	1.32
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	13	1.32
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	13	1.32
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	14	1.32
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	9	1.31
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	9	1.31
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	7	1.31
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	5	1.31
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	5	1.31
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	5	1.31
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	5	1.31
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	5	1.31
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	5	1.31
(1,331)	1:36:A:LEU:HD21	1:39:A:LEU:HD22	1	1.31
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	6	1.31
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	6	1.31
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	6	1.31
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	6	1.31
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	6	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	12	1.3
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	13	1.3
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	13	1.3
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	13	1.3
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	13	1.3
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	11	1.3
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	11	1.3
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	11	1.3
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	11	1.3
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	11	1.3
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	9	1.29
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	1	1.29
(1,755)	1:71:A:LEU:HD21	1:74:A:GLU:HG2	1	1.29
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	15	1.29
(1,498)	1:51:A:LEU:HD11	1:55:A:VAL:HG11	11	1.29
(1,498)	1:51:A:LEU:HD12	1:55:A:VAL:HG11	11	1.29
(1,498)	1:51:A:LEU:HD13	1:55:A:VAL:HG11	11	1.29
(1,491)	1:51:A:LEU:HD22	1:54:A:ARG:HA	15	1.29
(1,491)	1:51:A:LEU:HD23	1:54:A:ARG:HA	15	1.29
(1,489)	1:51:A:LEU:HD11	1:54:A:ARG:HA	11	1.29
(1,489)	1:51:A:LEU:HD12	1:54:A:ARG:HA	11	1.29
(1,489)	1:51:A:LEU:HD13	1:54:A:ARG:HA	11	1.29
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	14	1.29
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	5	1.29
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	5	1.29
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	5	1.29
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	10	1.29
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	13	1.28
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	15	1.28
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD22	1	1.28
(1,834)	1:88:A:SER:HA	1:89:A:LEU:HD23	1	1.28
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	5	1.28
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	5	1.28
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	5	1.28
(1,600)	1:58:A:VAL:HG13	1:96:A:LEU:HD21	14	1.28
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	13	1.28
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	1	1.28
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	2	1.28
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	13	1.28
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	9	1.28
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	7	1.27
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	5	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	9	1.27
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	9	1.27
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	9	1.27
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	9	1.27
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	9	1.27
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	9	1.27
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	10	1.27
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	10	1.27
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	10	1.27
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	10	1.27
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	10	1.27
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	10	1.27
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	1	1.27
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	4	1.27
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	9	1.27
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	1	1.26
(1,982)	1:100:A:LEU:HD21	1:102:A:GLU:H	3	1.26
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	15	1.26
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	9	1.26
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	14	1.26
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	12	1.26
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	2	1.26
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	15	1.26
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	15	1.26
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	15	1.26
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	15	1.26
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	15	1.26
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	1	1.26
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	1	1.26
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	15	1.26
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	15	1.26
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	2	1.26
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	3	1.26
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	3	1.26
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	3	1.26
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	10	1.26
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	10	1.26
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	10	1.26
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	10	1.26
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	10	1.26
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	12	1.26
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	12	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	12	1.26
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	12	1.26
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	12	1.26
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	14	1.25
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	14	1.25
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	14	1.25
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	10	1.25
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	6	1.25
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	6	1.25
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	6	1.25
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	5	1.25
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	5	1.25
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	5	1.25
(1,721)	1:67:A:SER:HA	1:71:A:LEU:HD21	1	1.25
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	15	1.25
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	11	1.25
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	8	1.25
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	7	1.25
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	8	1.25
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	8	1.25
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	8	1.25
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	2	1.25
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	3	1.24
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	3	1.24
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	5	1.24
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	10	1.24
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	10	1.24
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	10	1.24
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	10	1.24
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	10	1.24
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	8	1.24
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	1	1.24
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	2	1.24
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	2	1.24
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	2	1.24
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	2	1.24
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	2	1.24
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	5	1.24
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	5	1.24
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	5	1.24
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	13	1.24
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	6	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	14	1.24
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	15	1.23
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	10	1.23
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	10	1.23
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	2	1.23
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	9	1.23
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	9	1.23
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	7	1.23
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	13	1.23
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	14	1.23
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	14	1.23
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	14	1.23
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	1	1.23
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	5	1.23
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	3	1.23
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	6	1.23
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	5	1.22
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	4	1.22
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	14	1.22
(1,851)	1:89:A:LEU:HD22	1:91:A:ALA:H	2	1.22
(1,851)	1:89:A:LEU:HD23	1:91:A:ALA:H	2	1.22
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	11	1.22
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	11	1.22
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	7	1.22
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	7	1.22
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	7	1.22
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	7	1.22
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	7	1.22
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	7	1.22
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	9	1.22
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	4	1.22
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	4	1.22
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	15	1.22
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	15	1.22
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	15	1.22
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	15	1.22
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	15	1.22
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	10	1.22
(1,1053)	1:103:A:VAL:HA	1:106:A:LYS:HA	10	1.21
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	6	1.21
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	15	1.21
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	8	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	1:58:A:VAL:HG21	1:96:A:LEU:HD21	15	1.21
(1,588)	1:58:A:VAL:HG21	1:61:A:LEU:HD21	12	1.21
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	5	1.21
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	5	1.21
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	5	1.21
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	5	1.21
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	5	1.21
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	5	1.21
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	4	1.21
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	4	1.21
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	4	1.21
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	12	1.21
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	12	1.21
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	12	1.21
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	7	1.21
(1,982)	1:100:A:LEU:HD21	1:102:A:GLU:H	2	1.2
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	6	1.2
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	7	1.2
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	8	1.2
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	8	1.2
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG13	13	1.2
(1,784)	1:76:A:GLY:H	1:79:A:ILE:HG12	13	1.2
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	6	1.2
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	6	1.2
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	6	1.2
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG12	13	1.2
(1,771)	1:76:A:GLY:H	1:79:A:ILE:HG13	13	1.2
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	5	1.2
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	13	1.2
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	2	1.2
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	15	1.2
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	14	1.2
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	14	1.2
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	14	1.2
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	12	1.19
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	3	1.19
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	3	1.19
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	3	1.19
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	12	1.19
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	14	1.19
(1,721)	1:67:A:SER:HA	1:71:A:LEU:HD21	13	1.19
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	15	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	15	1.19
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	6	1.18
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	6	1.18
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	6	1.18
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	8	1.18
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	7	1.18
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	14	1.18
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	6	1.18
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	6	1.18
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	7	1.18
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	7	1.18
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	4	1.17
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	8	1.17
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	9	1.17
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	1	1.17
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	1	1.17
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	7	1.17
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	7	1.17
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	7	1.17
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	4	1.17
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	10	1.17
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	3	1.17
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	3	1.17
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	1	1.17
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	15	1.17
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	5	1.16
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	1	1.16
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	13	1.16
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	13	1.16
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	13	1.16
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	13	1.16
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	13	1.16
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	13	1.16
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	13	1.16
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	13	1.16
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	13	1.16
(1,606)	1:58:A:VAL:HG23	1:96:A:LEU:HD21	13	1.16
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	8	1.16
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	8	1.16
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	9	1.16
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	6	1.16
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	6	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD22	5	1.16
(1,256)	1:31:A:GLN:HG3	1:34:A:LEU:HD23	5	1.16
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD11	5	1.16
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD12	5	1.16
(1,256)	1:31:A:GLN:HG2	1:34:A:LEU:HD13	5	1.16
(1,66)	1:19:A:TRP:HA	1:23:A:VAL:H	15	1.16
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	3	1.16
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	12	1.15
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	4	1.15
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	4	1.15
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	4	1.15
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	9	1.15
(1,602)	1:58:A:VAL:HG21	1:96:A:LEU:HD21	1	1.15
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	6	1.15
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	9	1.15
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	9	1.15
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	13	1.15
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	13	1.15
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	13	1.15
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	13	1.15
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	13	1.15
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	13	1.15
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	13	1.15
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	13	1.15
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	4	1.14
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	14	1.14
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	13	1.14
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	7	1.14
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	14	1.14
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	7	1.14
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	7	1.14
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	7	1.14
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	5	1.14
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	5	1.14
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	5	1.14
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	11	1.14
(1,604)	1:58:A:VAL:HG22	1:96:A:LEU:HD21	15	1.14
(1,586)	1:58:A:VAL:HG13	1:61:A:LEU:HD21	12	1.14
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	4	1.14
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	4	1.14
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	13	1.14
(1,405)	1:42:A:MET:H	1:43:A:LEU:HG	3	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	3	1.14
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	3	1.14
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	11	1.14
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	11	1.14
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	1	1.14
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	1	1.14
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	13	1.13
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	9	1.13
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	9	1.13
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	7	1.13
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	7	1.13
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	2	1.13
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	2	1.13
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	2	1.13
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	2	1.13
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	2	1.13
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	2	1.13
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	11	1.13
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	15	1.13
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	14	1.13
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	14	1.13
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	14	1.13
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	2	1.13
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	2	1.13
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	7	1.13
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	7	1.13
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	7	1.13
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	12	1.13
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	9	1.13
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	9	1.13
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	9	1.13
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	2	1.13
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	11	1.12
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	13	1.12
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	13	1.12
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	13	1.12
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	13	1.12
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	13	1.12
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	13	1.12
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	13	1.12
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	12	1.12
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	4	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	4	1.12
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	4	1.12
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	15	1.12
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	7	1.12
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	7	1.12
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	9	1.12
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	7	1.12
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	13	1.12
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	10	1.12
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	10	1.12
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	10	1.12
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	10	1.11
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	3	1.11
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	4	1.11
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	10	1.11
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	15	1.11
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	15	1.11
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	15	1.11
(1,666)	1:61:A:LEU:HD11	1:96:A:LEU:HD22	9	1.11
(1,666)	1:61:A:LEU:HD12	1:96:A:LEU:HD22	9	1.11
(1,666)	1:61:A:LEU:HD13	1:96:A:LEU:HD22	9	1.11
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	1	1.11
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	1	1.11
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	1	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	1	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	1	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	1	1.11
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	6	1.11
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	6	1.11
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	6	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	6	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	6	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	6	1.11
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	7	1.11
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	7	1.11
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	7	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	7	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	7	1.11
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	7	1.11
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	8	1.11
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	3	1.11
(1,400)	1:41:A:LEU:HD21	1:42:A:MET:H	2	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	8	1.1
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	8	1.1
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	8	1.1
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	8	1.1
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	8	1.1
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	8	1.1
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	6	1.1
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	4	1.1
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	2	1.1
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	2	1.1
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	2	1.1
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	7	1.1
(1,604)	1:58:A:VAL:HG22	1:96:A:LEU:HD21	14	1.1
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	10	1.1
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	10	1.1
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	11	1.1
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	9	1.1
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	12	1.1
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	14	1.1
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	12	1.1
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	2	1.1
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	9	1.09
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	2	1.09
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	13	1.09
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	13	1.09
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	15	1.09
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	12	1.09
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	8	1.09
(1,833)	1:88:A:SER:HA	1:89:A:LEU:HD21	1	1.09
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	15	1.09
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	15	1.09
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	15	1.09
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	9	1.09
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	6	1.09
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	8	1.09
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	3	1.09
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	6	1.09
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	1	1.09
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	1	1.09
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	8	1.09
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	8	1.09
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	12	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	6	1.09
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	7	1.08
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	13	1.08
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	5	1.08
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	5	1.08
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	5	1.08
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	6	1.08
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	6	1.08
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	6	1.08
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	7	1.08
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	7	1.08
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	13	1.08
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	13	1.08
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	12	1.08
(1,600)	1:58:A:VAL:HG13	1:96:A:LEU:HD21	15	1.08
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	13	1.08
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	13	1.08
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	13	1.08
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	13	1.08
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	11	1.08
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	11	1.08
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	11	1.08
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	4	1.08
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	14	1.08
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	9	1.08
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	1	1.07
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	6	1.07
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	6	1.07
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	12	1.07
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	12	1.07
(1,602)	1:58:A:VAL:HG21	1:96:A:LEU:HD21	3	1.07
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	3	1.07
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	7	1.07
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	7	1.07
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	4	1.07
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	7	1.07
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	7	1.07
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	7	1.07
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	13	1.07
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	13	1.06
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	13	1.06
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	13	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	13	1.06
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	13	1.06
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	13	1.06
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	11	1.06
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	12	1.06
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	12	1.06
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	12	1.06
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	14	1.06
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	4	1.06
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	4	1.06
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	4	1.06
(1,400)	1:41:A:LEU:HD21	1:42:A:MET:H	3	1.06
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	14	1.06
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	14	1.06
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	14	1.06
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	14	1.06
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	14	1.06
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	12	1.06
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	12	1.06
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	10	1.05
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	10	1.05
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	6	1.05
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	1	1.05
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	1	1.05
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	3	1.05
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	3	1.05
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	15	1.05
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	15	1.05
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	3	1.05
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	3	1.05
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	3	1.05
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	5	1.05
(1,563)	1:57:A:ILE:HG23	1:61:A:LEU:HD21	14	1.05
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	3	1.05
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	3	1.05
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	3	1.05
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	3	1.05
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	3	1.05
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	3	1.05
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	14	1.05
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	10	1.05
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	14	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	9	1.05
(1,331)	1:36:A:LEU:HD21	1:39:A:LEU:HD22	2	1.05
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD11	15	1.05
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD12	15	1.05
(1,254)	1:31:A:GLN:HG3	1:34:A:LEU:HD13	15	1.05
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	14	1.05
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	12	1.05
(1,84)	1:20:A:LEU:HD11	1:23:A:VAL:HG11	6	1.05
(1,84)	1:20:A:LEU:HD12	1:23:A:VAL:HG11	6	1.05
(1,84)	1:20:A:LEU:HD13	1:23:A:VAL:HG11	6	1.05
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	14	1.04
(1,864)	1:89:A:LEU:HD21	1:92:A:ALA:HB3	10	1.04
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	8	1.04
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	8	1.04
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	8	1.04
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	7	1.04
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	13	1.04
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	13	1.04
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	13	1.04
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	13	1.04
(1,598)	1:58:A:VAL:HG12	1:96:A:LEU:HD21	13	1.04
(1,588)	1:58:A:VAL:HG21	1:61:A:LEU:HD21	13	1.04
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	3	1.04
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	3	1.04
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG21	13	1.04
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG21	13	1.04
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG21	13	1.04
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG22	13	1.04
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG22	13	1.04
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG22	13	1.04
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG23	13	1.04
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG23	13	1.04
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG23	13	1.04
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	9	1.04
(1,382)	1:39:A:LEU:HG	1:40:A:ASN:H	10	1.04
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	13	1.04
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	13	1.04
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	13	1.04
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	13	1.04
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	13	1.04
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	8	1.04
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	10	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	6	1.04
(1,721)	1:67:A:SER:HA	1:71:A:LEU:HD21	15	1.03
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	13	1.03
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	15	1.03
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	15	1.03
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	15	1.03
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	8	1.03
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	13	1.03
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	13	1.03
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	13	1.03
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	15	1.03
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	15	1.03
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	15	1.03
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	10	1.02
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	4	1.02
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	6	1.02
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	8	1.02
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	12	1.02
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	8	1.01
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	8	1.01
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	2	1.01
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	12	1.01
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	5	1.01
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	1	1.01
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	12	1.01
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	13	1.01
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	7	1.01
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	7	1.01
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	7	1.01
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	9	1.01
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	8	1.0
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	14	1.0
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	2	1.0
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	14	1.0
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	8	1.0
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	8	1.0
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	10	1.0
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	10	1.0
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	3	1.0
(1,368)	1:38:A:LEU:HD21	1:41:A:LEU:H	10	1.0
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	10	1.0
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	5	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	4	1.0
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	10	1.0
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	2	0.99
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	7	0.99
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	10	0.99
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	10	0.99
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	10	0.99
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	12	0.99
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	12	0.99
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	10	0.99
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	5	0.99
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	5	0.99
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	7	0.99
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	5	0.99
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	5	0.99
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	5	0.99
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	5	0.99
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	5	0.99
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	5	0.99
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	10	0.99
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	10	0.99
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	10	0.99
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	1	0.99
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	3	0.99
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	14	0.99
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	14	0.99
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	14	0.99
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	14	0.99
(1,977)	1:100:A:LEU:HG	1:101:A:GLU:H	2	0.98
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	9	0.98
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	9	0.98
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	9	0.98
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	13	0.98
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	4	0.98
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	4	0.98
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	4	0.98
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	13	0.98
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	2	0.98
(1,707)	1:66:A:MET:HB3	1:68:A:GLN:HB3	6	0.98
(1,707)	1:66:A:MET:HB3	1:68:A:GLN:HB2	6	0.98
(1,707)	1:66:A:MET:HB2	1:68:A:GLN:HB3	6	0.98
(1,707)	1:66:A:MET:HB2	1:68:A:GLN:HB2	6	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:51:A:LEU:HD21	1:55:A:VAL:HG21	2	0.98
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	4	0.98
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	4	0.98
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	4	0.98
(1,84)	1:20:A:LEU:HD11	1:23:A:VAL:HG11	5	0.98
(1,84)	1:20:A:LEU:HD12	1:23:A:VAL:HG11	5	0.98
(1,84)	1:20:A:LEU:HD13	1:23:A:VAL:HG11	5	0.98
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	7	0.97
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	9	0.97
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	9	0.97
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	14	0.97
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	14	0.97
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	1	0.97
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	9	0.97
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	6	0.97
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	6	0.97
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD22	12	0.97
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD23	12	0.97
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	8	0.97
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	8	0.97
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	8	0.97
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	14	0.97
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	3	0.97
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	12	0.97
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	11	0.97
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	8	0.96
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	8	0.96
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	8	0.96
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	8	0.96
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	8	0.96
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	8	0.96
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	15	0.96
(1,974)	1:99:A:TRP:HA	1:103:A:VAL:H	9	0.96
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	2	0.96
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	14	0.96
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	14	0.96
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	13	0.96
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	13	0.96
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	13	0.96
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	15	0.96
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	4	0.96
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	4	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	4	0.96
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	4	0.96
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	11	0.96
(1,210)	1:27:A:LYS:HD3	1:28:A:ASN:H	9	0.96
(1,210)	1:27:A:LYS:HD2	1:28:A:ASN:H	9	0.96
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	10	0.96
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	7	0.96
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	7	0.96
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	7	0.96
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	10	0.96
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	10	0.96
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	10	0.96
(1,71)	1:19:A:TRP:H	1:20:A:LEU:HD21	15	0.96
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	9	0.96
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	13	0.95
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	13	0.95
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	10	0.95
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	10	0.95
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	10	0.95
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	10	0.95
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	10	0.95
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	10	0.95
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	5	0.95
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	5	0.95
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	5	0.95
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	8	0.95
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	8	0.95
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	7	0.95
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	14	0.95
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	14	0.95
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	14	0.95
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	3	0.95
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	3	0.95
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	7	0.95
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	7	0.95
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	7	0.95
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	7	0.95
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	4	0.95
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD22	2	0.95
(1,579)	1:58:A:VAL:HB	1:61:A:LEU:HD23	2	0.95
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	9	0.95
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	9	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	9	0.95
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	11	0.95
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	11	0.95
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	11	0.95
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	10	0.95
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	10	0.95
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	3	0.95
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	3	0.95
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	11	0.95
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	3	0.95
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	3	0.95
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	3	0.95
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	13	0.95
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	6	0.95
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	10	0.94
(1,939)	1:96:A:LEU:HD13	1:100:A:LEU:HD21	15	0.94
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	15	0.94
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	15	0.94
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	15	0.94
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	10	0.94
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	10	0.94
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	10	0.94
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	7	0.94
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	7	0.94
(1,721)	1:67:A:SER:HA	1:71:A:LEU:HD21	3	0.94
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	11	0.94
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	14	0.94
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	1	0.94
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	10	0.94
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	10	0.94
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	10	0.94
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	10	0.94
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	10	0.94
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	10	0.94
(1,503)	1:51:A:LEU:HD21	1:55:A:VAL:HG13	6	0.94
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	9	0.94
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	1	0.94
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	9	0.94
(1,212)	1:27:A:LYS:H	1:30:A:TYR:HD1	15	0.94
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	13	0.94
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	13	0.94
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	1	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	1	0.94
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	1	0.94
(1,1008)	1:101:A:GLU:HA	1:105:A:LEU:H	4	0.93
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	8	0.93
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	11	0.93
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	1	0.93
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	10	0.93
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	10	0.93
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	10	0.93
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	11	0.93
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	11	0.93
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	11	0.93
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	12	0.93
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	9	0.93
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	9	0.93
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	9	0.93
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	9	0.93
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	9	0.93
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	13	0.93
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	3	0.93
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	3	0.93
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	3	0.93
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	3	0.93
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	3	0.93
(1,331)	1:36:A:LEU:HD21	1:39:A:LEU:HD22	3	0.93
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	6	0.93
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	15	0.92
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	7	0.92
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	7	0.92
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	12	0.92
(1,864)	1:89:A:LEU:HD21	1:92:A:ALA:HB3	12	0.92
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	6	0.92
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	1	0.92
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	1	0.92
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	1	0.92
(1,819)	1:84:A:ARG:HB3	1:86:A:SER:HA	2	0.92
(1,819)	1:84:A:ARG:HB2	1:86:A:SER:HA	2	0.92
(1,777)	1:77:A:ALA:HA	1:79:A:ILE:H	10	0.92
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	13	0.92
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	8	0.92
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	11	0.92
(1,600)	1:58:A:VAL:HG13	1:96:A:LEU:HD21	10	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG21	7	0.92
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG21	7	0.92
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG21	7	0.92
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG22	7	0.92
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG22	7	0.92
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG22	7	0.92
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG23	7	0.92
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG23	7	0.92
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG23	7	0.92
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	12	0.92
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	3	0.92
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	5	0.92
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	3	0.92
(1,333)	1:36:A:LEU:HD21	1:39:A:LEU:HD23	1	0.92
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	4	0.92
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	4	0.92
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	3	0.91
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	9	0.91
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	2	0.91
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	2	0.91
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	11	0.91
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	11	0.91
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	11	0.91
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	11	0.91
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	11	0.91
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	11	0.91
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	11	0.91
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	11	0.91
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	11	0.91
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	11	0.91
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	8	0.91
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	8	0.91
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	8	0.91
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	2	0.91
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	2	0.91
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	10	0.91
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	4	0.91
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	4	0.91
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	9	0.91
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	9	0.91
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	9	0.91
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	11	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	14	0.91
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD22	14	0.91
(1,347)	1:37:A:PRO:HA	1:38:A:LEU:HD23	14	0.91
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	6	0.91
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	2	0.91
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	2	0.91
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	4	0.9
(1,982)	1:100:A:LEU:HD21	1:102:A:GLU:H	15	0.9
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	11	0.9
(1,885)	1:92:A:ALA:HB1	1:94:A:VAL:HB	6	0.9
(1,885)	1:92:A:ALA:HB2	1:94:A:VAL:HB	6	0.9
(1,885)	1:92:A:ALA:HB3	1:94:A:VAL:HB	6	0.9
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	15	0.9
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	14	0.9
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	14	0.9
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	14	0.9
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	13	0.9
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	2	0.9
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	2	0.9
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	2	0.9
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	2	0.9
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	2	0.9
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	8	0.9
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	9	0.9
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	12	0.9
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	4	0.9
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	13	0.9
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	13	0.9
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	7	0.9
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	13	0.9
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	4	0.89
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	12	0.89
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	11	0.89
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	3	0.89
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	7	0.89
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	7	0.89
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	7	0.89
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	12	0.89
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	12	0.89
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	12	0.89
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	11	0.89
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	11	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	11	0.89
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	5	0.89
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	15	0.89
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	4	0.89
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	4	0.89
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	4	0.89
(1,563)	1:57:A:ILE:HG23	1:61:A:LEU:HD21	11	0.89
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	4	0.89
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	6	0.89
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	6	0.89
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	6	0.89
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	6	0.89
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	6	0.89
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	4	0.89
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	9	0.89
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	9	0.89
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	12	0.89
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	12	0.89
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	12	0.89
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	8	0.89
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	10	0.89
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	6	0.88
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	6	0.88
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	6	0.88
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	6	0.88
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	6	0.88
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	6	0.88
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	10	0.88
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	13	0.88
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	13	0.88
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	2	0.88
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	2	0.88
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	11	0.88
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	1	0.88
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	13	0.88
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	8	0.88
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	8	0.88
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	8	0.88
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	8	0.88
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	8	0.88
(1,283)	1:33:A:ASP:HA	1:36:A:LEU:HD21	13	0.88
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	13	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	13	0.88
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	2	0.88
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	4	0.87
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	4	0.87
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	4	0.87
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	3	0.87
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	3	0.87
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	11	0.87
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	5	0.87
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	9	0.87
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	15	0.87
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	1	0.87
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	1	0.87
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	12	0.87
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	8	0.87
(1,270)	1:32:A:ASN:HB3	1:34:A:LEU:HD21	7	0.87
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	2	0.87
(1,210)	1:27:A:LYS:HD3	1:28:A:ASN:H	4	0.87
(1,210)	1:27:A:LYS:HD2	1:28:A:ASN:H	4	0.87
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	3	0.87
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	8	0.86
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	8	0.86
(1,606)	1:58:A:VAL:HG23	1:96:A:LEU:HD21	11	0.86
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	9	0.86
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	8	0.86
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	7	0.85
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	5	0.85
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	15	0.85
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	4	0.85
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	4	0.85
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	3	0.85
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	3	0.85
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	1	0.85
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	10	0.85
(1,604)	1:58:A:VAL:HG22	1:96:A:LEU:HD21	9	0.85
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	4	0.85
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	4	0.85
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	4	0.85
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	4	0.85
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	4	0.85
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	4	0.85
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	8	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	8	0.85
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	8	0.85
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	8	0.85
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	8	0.85
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	8	0.85
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	12	0.85
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	13	0.85
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	10	0.85
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	10	0.85
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	10	0.85
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	10	0.85
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	10	0.85
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	12	0.85
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	12	0.85
(1,210)	1:27:A:LYS:HD3	1:28:A:ASN:H	5	0.85
(1,210)	1:27:A:LYS:HD2	1:28:A:ASN:H	5	0.85
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	7	0.85
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	12	0.85
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	11	0.85
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	2	0.84
(1,982)	1:100:A:LEU:HD21	1:102:A:GLU:H	5	0.84
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	10	0.84
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	14	0.84
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	1	0.84
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	9	0.84
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	12	0.84
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	14	0.84
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	10	0.84
(1,400)	1:41:A:LEU:HD21	1:42:A:MET:H	11	0.84
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	4	0.84
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	8	0.84
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	3	0.84
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	15	0.84
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	8	0.83
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	2	0.83
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	2	0.83
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	2	0.83
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	2	0.83
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	2	0.83
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	2	0.83
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	5	0.83
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	5	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	5	0.83
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	5	0.83
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	5	0.83
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	5	0.83
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	9	0.83
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	9	0.83
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	9	0.83
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	5	0.83
(1,559)	1:57:A:ILE:HG21	1:61:A:LEU:HD21	6	0.83
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	5	0.83
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	5	0.83
(1,66)	1:19:A:TRP:HA	1:23:A:VAL:H	14	0.83
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	5	0.82
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	1	0.82
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	11	0.82
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	9	0.82
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	5	0.82
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	3	0.82
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	3	0.82
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	3	0.82
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	3	0.82
(1,721)	1:67:A:SER:HA	1:71:A:LEU:HD21	5	0.82
(1,600)	1:58:A:VAL:HG13	1:96:A:LEU:HD21	12	0.82
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	5	0.82
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	5	0.82
(1,501)	1:51:A:LEU:HD21	1:55:A:VAL:HG12	11	0.82
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	2	0.82
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	2	0.82
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	2	0.82
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	14	0.82
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	9	0.82
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	14	0.82
(1,329)	1:36:A:LEU:HD22	1:39:A:LEU:HD21	12	0.82
(1,329)	1:36:A:LEU:HD23	1:39:A:LEU:HD21	12	0.82
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	14	0.82
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	5	0.81
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	13	0.81
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	13	0.81
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	7	0.81
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	7	0.81
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	7	0.81
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	7	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	7	0.81
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	7	0.81
(1,857)	1:89:A:LEU:HD21	1:92:A:ALA:H	3	0.81
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	13	0.81
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	13	0.81
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	13	0.81
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	15	0.81
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	1	0.81
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	1	0.81
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	1	0.81
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	2	0.81
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	5	0.81
(1,210)	1:27:A:LYS:HD3	1:28:A:ASN:H	10	0.81
(1,210)	1:27:A:LYS:HD2	1:28:A:ASN:H	10	0.81
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	10	0.81
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	9	0.81
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	9	0.81
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	9	0.81
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	12	0.81
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	6	0.8
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	6	0.8
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	5	0.8
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	5	0.8
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	4	0.8
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	13	0.8
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	7	0.8
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	7	0.8
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	7	0.8
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	7	0.8
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	7	0.8
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	2	0.8
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	11	0.8
(1,19)	1:15:A:ARG:HG3	1:19:A:TRP:H	7	0.8
(1,19)	1:15:A:ARG:HG2	1:19:A:TRP:H	7	0.8
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	9	0.79
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	9	0.79
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	6	0.79
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	12	0.79
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	14	0.79
(1,982)	1:100:A:LEU:HD21	1:102:A:GLU:H	14	0.79
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	2	0.79
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	9	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	11	0.79
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	11	0.79
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	4	0.79
(1,860)	1:89:A:LEU:HD21	1:92:A:ALA:HB1	4	0.79
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	11	0.79
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	8	0.79
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	8	0.79
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	8	0.79
(1,592)	1:58:A:VAL:HG23	1:61:A:LEU:HD21	6	0.79
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	7	0.79
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	10	0.79
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	10	0.79
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	10	0.79
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	6	0.79
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	11	0.79
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	2	0.78
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	2	0.78
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	2	0.78
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	2	0.78
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	2	0.78
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	2	0.78
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	13	0.78
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	15	0.78
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	14	0.78
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	7	0.78
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	7	0.78
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	7	0.78
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	3	0.78
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	5	0.78
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	9	0.78
(1,606)	1:58:A:VAL:HG23	1:96:A:LEU:HD21	12	0.78
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	10	0.78
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	10	0.78
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	10	0.78
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	10	0.78
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	10	0.78
(1,491)	1:51:A:LEU:HD22	1:54:A:ARG:HA	7	0.78
(1,491)	1:51:A:LEU:HD23	1:54:A:ARG:HA	7	0.78
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	4	0.78
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	2	0.78
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	3	0.78
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	11	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	15	0.78
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	15	0.78
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	15	0.78
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD22	10	0.78
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD23	10	0.78
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	9	0.78
(1,1083)	1:106:A:LYS:HG3	1:108:A:ASP:H	3	0.77
(1,1083)	1:106:A:LYS:HG2	1:108:A:ASP:H	3	0.77
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	14	0.77
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	11	0.77
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	8	0.77
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	4	0.77
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	9	0.77
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	12	0.77
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	12	0.77
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	12	0.77
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	12	0.77
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	12	0.77
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	12	0.77
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	3	0.77
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	3	0.77
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	3	0.77
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	7	0.77
(1,592)	1:58:A:VAL:HG23	1:61:A:LEU:HD21	12	0.77
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	15	0.77
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	15	0.77
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	15	0.77
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	15	0.77
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	6	0.77
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	6	0.77
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	9	0.77
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	8	0.77
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	4	0.77
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	4	0.77
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	4	0.77
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	6	0.77
(1,1026)	1:103:A:VAL:H	1:104:A:LEU:HD21	15	0.76
(1,945)	1:96:A:LEU:HD22	1:100:A:LEU:HD21	12	0.76
(1,801)	1:81:A:THR:HA	1:84:A:ARG:H	15	0.76
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	11	0.76
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	15	0.76
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	15	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	15	0.76
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	15	0.76
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	4	0.76
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	8	0.76
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	8	0.76
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	8	0.76
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	8	0.76
(1,588)	1:58:A:VAL:HG21	1:61:A:LEU:HD21	11	0.76
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	9	0.76
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	9	0.76
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	9	0.76
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	9	0.76
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	9	0.76
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	9	0.76
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	9	0.76
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	6	0.76
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	8	0.76
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	14	0.76
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	6	0.76
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	15	0.76
(1,1026)	1:103:A:VAL:H	1:104:A:LEU:HD21	13	0.75
(1,923)	1:96:A:LEU:HD21	1:98:A:GLN:H	1	0.75
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	3	0.75
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	3	0.75
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	2	0.75
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	4	0.75
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	4	0.75
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	4	0.75
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	4	0.75
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	4	0.75
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	4	0.75
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD11	3	0.75
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD12	3	0.75
(1,832)	1:88:A:SER:HA	1:89:A:LEU:HD13	3	0.75
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	11	0.75
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	11	0.75
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	11	0.75
(1,786)	1:78:A:GLY:H	1:81:A:THR:H	7	0.75
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	4	0.75
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	4	0.75
(1,341)	1:37:A:PRO:HD2	1:38:A:LEU:HD21	12	0.75
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	15	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	7	0.75
(1,942)	1:96:A:LEU:HD21	1:100:A:LEU:HD21	10	0.74
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	9	0.74
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	8	0.74
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	8	0.74
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	15	0.74
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	15	0.74
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	15	0.74
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	10	0.74
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	3	0.74
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	14	0.74
(1,462)	1:50:A:ALA:HB1	1:51:A:LEU:HD21	9	0.74
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	4	0.74
(1,329)	1:36:A:LEU:HD22	1:39:A:LEU:HD21	14	0.74
(1,329)	1:36:A:LEU:HD23	1:39:A:LEU:HD21	14	0.74
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	12	0.74
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	15	0.74
(1,19)	1:15:A:ARG:HG3	1:19:A:TRP:H	3	0.74
(1,19)	1:15:A:ARG:HG2	1:19:A:TRP:H	3	0.74
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	9	0.73
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	9	0.73
(1,965)	1:98:A:GLN:HA	1:101:A:GLU:H	5	0.73
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	5	0.73
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	2	0.73
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	9	0.73
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	9	0.73
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	14	0.73
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	14	0.73
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	6	0.73
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	10	0.73
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	14	0.73
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	14	0.73
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	14	0.73
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	14	0.73
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	14	0.73
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	4	0.73
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	4	0.73
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	4	0.73
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	2	0.73
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	11	0.73
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD22	2	0.73
(1,359)	1:37:A:PRO:HB2	1:41:A:LEU:HD23	2	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:36:A:LEU:HD21	1:39:A:LEU:HD23	2	0.73
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD22	12	0.73
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD23	12	0.73
(1,66)	1:19:A:TRP:HA	1:23:A:VAL:H	8	0.73
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	11	0.72
(1,982)	1:100:A:LEU:HD21	1:102:A:GLU:H	4	0.72
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	2	0.72
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	2	0.72
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	3	0.72
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	3	0.72
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	3	0.72
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	3	0.72
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	3	0.72
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	3	0.72
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	9	0.72
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	9	0.72
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	9	0.72
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	12	0.72
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	12	0.72
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	12	0.72
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	8	0.72
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	8	0.72
(1,722)	1:67:A:SER:HA	1:71:A:LEU:HD22	13	0.72
(1,722)	1:67:A:SER:HA	1:71:A:LEU:HD23	13	0.72
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	6	0.72
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	1	0.72
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	1	0.72
(1,582)	1:58:A:VAL:HG11	1:61:A:LEU:HD21	15	0.72
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	11	0.72
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	11	0.72
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	11	0.72
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	11	0.72
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	11	0.72
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	11	0.72
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	6	0.72
(1,69)	1:19:A:TRP:H	1:20:A:LEU:HG	10	0.72
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	3	0.72
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	13	0.71
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	3	0.71
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	13	0.71
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	13	0.71
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	13	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	3	0.71
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	13	0.71
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	8	0.71
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	8	0.71
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	8	0.71
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	9	0.71
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	14	0.71
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	5	0.71
(1,1022)	1:102:A:GLU:HA	1:106:A:LYS:H	4	0.7
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	14	0.7
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	3	0.7
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	12	0.7
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	5	0.7
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	14	0.7
(1,588)	1:58:A:VAL:HG21	1:61:A:LEU:HD21	7	0.7
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	7	0.7
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	7	0.7
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	7	0.7
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	7	0.7
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	7	0.7
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	7	0.7
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	13	0.7
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	8	0.7
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	8	0.7
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	8	0.7
(1,462)	1:50:A:ALA:HB1	1:51:A:LEU:HD21	8	0.7
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	6	0.7
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	1	0.7
(1,329)	1:36:A:LEU:HD22	1:39:A:LEU:HD21	8	0.7
(1,329)	1:36:A:LEU:HD23	1:39:A:LEU:HD21	8	0.7
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	13	0.7
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	4	0.7
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	7	0.7
(1,210)	1:27:A:LYS:HD3	1:28:A:ASN:H	7	0.7
(1,210)	1:27:A:LYS:HD2	1:28:A:ASN:H	7	0.7
(1,69)	1:19:A:TRP:H	1:20:A:LEU:HG	2	0.7
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	1	0.69
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	3	0.69
(1,945)	1:96:A:LEU:HD22	1:100:A:LEU:HD21	6	0.69
(1,933)	1:96:A:LEU:HD22	1:99:A:TRP:HB2	6	0.69
(1,933)	1:96:A:LEU:HD23	1:99:A:TRP:HB2	6	0.69
(1,895)	1:93:A:PRO:HG3	1:97:A:ARG:H	2	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,895)	1:93:A:PRO:HG2	1:97:A:ARG:H	2	0.69
(1,860)	1:89:A:LEU:HD21	1:92:A:ALA:HB1	5	0.69
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	8	0.69
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	8	0.69
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	8	0.69
(1,849)	1:89:A:LEU:HD11	1:91:A:ALA:H	14	0.69
(1,849)	1:89:A:LEU:HD12	1:91:A:ALA:H	14	0.69
(1,849)	1:89:A:LEU:HD13	1:91:A:ALA:H	14	0.69
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	11	0.69
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	11	0.69
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	11	0.69
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	10	0.69
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	10	0.69
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	14	0.69
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	6	0.69
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	2	0.69
(1,400)	1:41:A:LEU:HD21	1:42:A:MET:H	4	0.69
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	10	0.69
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	9	0.69
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	9	0.69
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	15	0.69
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	11	0.69
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	13	0.69
(1,1083)	1:106:A:LYS:HG3	1:108:A:ASP:H	2	0.68
(1,1083)	1:106:A:LYS:HG2	1:108:A:ASP:H	2	0.68
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	9	0.68
(1,945)	1:96:A:LEU:HD22	1:100:A:LEU:HD21	7	0.68
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	11	0.68
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	11	0.68
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	11	0.68
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	1	0.68
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG21	8	0.68
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG21	8	0.68
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG21	8	0.68
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG22	8	0.68
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG22	8	0.68
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG22	8	0.68
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG23	8	0.68
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG23	8	0.68
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG23	8	0.68
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG21	14	0.68
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG21	14	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG21	14	0.68
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG22	14	0.68
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG22	14	0.68
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG22	14	0.68
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG23	14	0.68
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG23	14	0.68
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG23	14	0.68
(1,441)	1:47:A:GLU:HA	1:49:A:GLU:H	5	0.68
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	10	0.68
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	14	0.68
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	2	0.68
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	6	0.68
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	6	0.68
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	6	0.68
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	1	0.68
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	10	0.67
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	10	0.67
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	10	0.67
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	10	0.67
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	10	0.67
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	10	0.67
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	3	0.67
(1,895)	1:93:A:PRO:HG3	1:97:A:ARG:H	13	0.67
(1,895)	1:93:A:PRO:HG2	1:97:A:ARG:H	13	0.67
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	11	0.67
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	11	0.67
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	13	0.67
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	8	0.67
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	8	0.67
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	8	0.67
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	8	0.67
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	8	0.67
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	8	0.67
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	8	0.67
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	8	0.67
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	8	0.67
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	11	0.67
(1,604)	1:58:A:VAL:HG22	1:96:A:LEU:HD21	10	0.67
(1,571)	1:58:A:VAL:HA	1:61:A:LEU:H	12	0.67
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	2	0.67
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	14	0.67
(1,330)	1:36:A:LEU:HD11	1:39:A:LEU:HD22	11	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:36:A:LEU:HD12	1:39:A:LEU:HD22	11	0.67
(1,330)	1:36:A:LEU:HD13	1:39:A:LEU:HD22	11	0.67
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	2	0.67
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	15	0.67
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	1	0.66
(1,942)	1:96:A:LEU:HD21	1:100:A:LEU:HD21	12	0.66
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	9	0.66
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	9	0.66
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	9	0.66
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	9	0.66
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	9	0.66
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	9	0.66
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	5	0.66
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	3	0.66
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG3	12	0.66
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG2	12	0.66
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	4	0.66
(1,509)	1:51:A:LEU:HD21	1:55:A:VAL:HG23	2	0.66
(1,497)	1:51:A:LEU:HA	1:55:A:VAL:H	14	0.66
(1,491)	1:51:A:LEU:HD22	1:54:A:ARG:HA	6	0.66
(1,491)	1:51:A:LEU:HD23	1:54:A:ARG:HA	6	0.66
(1,491)	1:51:A:LEU:HD22	1:54:A:ARG:HA	14	0.66
(1,491)	1:51:A:LEU:HD23	1:54:A:ARG:HA	14	0.66
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	13	0.66
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	2	0.66
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	2	0.66
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	3	0.66
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	5	0.66
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	5	0.66
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	12	0.66
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	12	0.66
(1,181)	1:25:A:LEU:HD22	1:28:A:ASN:HB2	1	0.66
(1,181)	1:25:A:LEU:HD23	1:28:A:ASN:HB2	1	0.66
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	8	0.66
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	8	0.66
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	8	0.66
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	2	0.66
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	8	0.65
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	1	0.65
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	1	0.65
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	4	0.65
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	7	0.65
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	5	0.65
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	5	0.65
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG3	14	0.65
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG2	14	0.65
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	7	0.65
(1,586)	1:58:A:VAL:HG13	1:61:A:LEU:HD21	6	0.65
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	15	0.65
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	15	0.65
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	15	0.65
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	15	0.65
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	15	0.65
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	3	0.65
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	3	0.65
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	3	0.65
(1,462)	1:50:A:ALA:HB1	1:51:A:LEU:HD21	12	0.65
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	4	0.65
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	4	0.65
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	3	0.65
(1,333)	1:36:A:LEU:HD21	1:39:A:LEU:HD23	3	0.65
(1,272)	1:32:A:ASN:HB2	1:34:A:LEU:HD21	7	0.65
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	11	0.65
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	11	0.65
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	11	0.65
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	6	0.65
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD22	2	0.65
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD23	2	0.65
(1,69)	1:19:A:TRP:H	1:20:A:LEU:HG	9	0.65
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	1	0.64
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	1	0.64
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	1	0.64
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	1	0.64
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	1	0.64
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	1	0.64
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	1	0.64
(1,860)	1:89:A:LEU:HD21	1:92:A:ALA:HB1	6	0.64
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	10	0.64
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	12	0.64
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	4	0.64
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	14	0.64
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	15	0.64
(1,142)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	10	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	10	0.64
(1,66)	1:19:A:TRP:HA	1:23:A:VAL:H	10	0.64
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	13	0.64
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	13	0.63
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	15	0.63
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	9	0.63
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	5	0.63
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	5	0.63
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	15	0.63
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	15	0.63
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	15	0.63
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	15	0.63
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	15	0.63
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	15	0.63
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	15	0.63
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	15	0.63
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	15	0.63
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	5	0.63
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	5	0.63
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	3	0.63
(1,559)	1:57:A:ILE:HG21	1:61:A:LEU:HD21	4	0.63
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	7	0.63
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	7	0.63
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	7	0.63
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	1	0.63
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	7	0.63
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	12	0.63
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	8	0.63
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	8	0.63
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	1	0.63
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	1	0.63
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	12	0.63
(1,223)	1:28:A:ASN:HA	1:32:A:ASN:H	14	0.63
(1,217)	1:27:A:LYS:HA	1:31:A:GLN:H	1	0.63
(1,148)	1:23:A:VAL:HG22	1:26:A:LEU:HD21	14	0.63
(1,142)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	3	0.63
(1,84)	1:20:A:LEU:HD11	1:23:A:VAL:HG11	12	0.63
(1,84)	1:20:A:LEU:HD12	1:23:A:VAL:HG11	12	0.63
(1,84)	1:20:A:LEU:HD13	1:23:A:VAL:HG11	12	0.63
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	7	0.63
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	7	0.63
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	7	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	3	0.63
(1,1083)	1:106:A:LYS:HG3	1:108:A:ASP:H	5	0.62
(1,1083)	1:106:A:LYS:HG2	1:108:A:ASP:H	5	0.62
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	8	0.62
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	8	0.62
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	8	0.62
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	5	0.62
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	5	0.62
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	12	0.62
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	12	0.62
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	12	0.62
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	12	0.62
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	12	0.62
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	12	0.62
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	4	0.62
(1,947)	1:96:A:LEU:HD23	1:100:A:LEU:HD21	6	0.62
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	6	0.62
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	9	0.62
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	9	0.62
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	9	0.62
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	8	0.62
(1,721)	1:67:A:SER:HA	1:71:A:LEU:HD21	14	0.62
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	3	0.62
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	3	0.62
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	6	0.62
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	6	0.62
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	6	0.62
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	6	0.62
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	2	0.62
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD22	1	0.62
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD23	1	0.62
(1,487)	1:51:A:LEU:HD21	1:54:A:ARG:H	2	0.62
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	13	0.62
(1,405)	1:42:A:MET:H	1:43:A:LEU:HG	2	0.62
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	5	0.62
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	12	0.62
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	12	0.62
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	12	0.62
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	12	0.62
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	12	0.62
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	10	0.62
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	10	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	10	0.62
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD22	7	0.62
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD23	7	0.62
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	1	0.62
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	1	0.62
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	13	0.62
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	9	0.62
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	13	0.62
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	1	0.62
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	7	0.61
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	7	0.61
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	1	0.61
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	1	0.61
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	1	0.61
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	1	0.61
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	1	0.61
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	1	0.61
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	15	0.61
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	15	0.61
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	15	0.61
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	13	0.61
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	13	0.61
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG3	13	0.61
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG2	13	0.61
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	12	0.61
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	11	0.61
(1,441)	1:47:A:GLU:HA	1:49:A:GLU:H	4	0.61
(1,441)	1:47:A:GLU:HA	1:49:A:GLU:H	12	0.61
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	2	0.61
(1,384)	1:39:A:LEU:HD21	1:40:A:ASN:H	8	0.61
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	3	0.6
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	7	0.6
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	4	0.6
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	4	0.6
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	4	0.6
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	2	0.6
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	2	0.6
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	3	0.6
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	3	0.6
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	9	0.6
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	2	0.6
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	1	0.6
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	1	0.6
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	1	0.6
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	1	0.6
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	1	0.6
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	1	0.6
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	12	0.6
(1,400)	1:41:A:LEU:HD21	1:42:A:MET:H	7	0.6
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	14	0.6
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	1	0.6
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	10	0.6
(1,69)	1:19:A:TRP:H	1:20:A:LEU:HG	11	0.6
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	5	0.59
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	5	0.59
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	5	0.59
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	4	0.59
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	5	0.59
(1,945)	1:96:A:LEU:HD22	1:100:A:LEU:HD21	5	0.59
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	10	0.59
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	8	0.59
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	8	0.59
(1,795)	1:80:A:ALA:HA	1:84:A:ARG:HA	3	0.59
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	1	0.59
(1,721)	1:67:A:SER:HA	1:71:A:LEU:HD21	12	0.59
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	7	0.59
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	2	0.59
(1,586)	1:58:A:VAL:HG13	1:61:A:LEU:HD21	11	0.59
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD22	13	0.59
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD23	13	0.59
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG21	10	0.59
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG21	10	0.59
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG21	10	0.59
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG22	10	0.59
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG22	10	0.59
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG22	10	0.59
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG23	10	0.59
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG23	10	0.59
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG23	10	0.59
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	6	0.59
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	6	0.59
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	6	0.59
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	6	0.59
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	6	0.59
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	5	0.59
(1,405)	1:42:A:MET:H	1:43:A:LEU:HG	12	0.59
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD22	15	0.59
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD23	15	0.59
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD22	9	0.59
(1,284)	1:33:A:ASP:HA	1:36:A:LEU:HD23	9	0.59
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD22	4	0.59
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD23	4	0.59
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	5	0.59
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	6	0.59
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD22	5	0.59
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD23	5	0.59
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	5	0.59
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	9	0.58
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	4	0.58
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	4	0.58
(1,753)	1:71:A:LEU:HD21	1:74:A:GLU:HG3	1	0.58
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	4	0.58
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	14	0.58
(1,675)	1:62:A:LEU:HD11	1:64:A:GLY:H	4	0.58
(1,675)	1:62:A:LEU:HD12	1:64:A:GLY:H	4	0.58
(1,675)	1:62:A:LEU:HD13	1:64:A:GLY:H	4	0.58
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	4	0.58
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG21	2	0.58
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG21	2	0.58
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG21	2	0.58
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG22	2	0.58
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG22	2	0.58
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG22	2	0.58
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG23	2	0.58
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG23	2	0.58
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG23	2	0.58
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	14	0.58
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	8	0.58
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	8	0.58
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	8	0.58
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	8	0.58
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	8	0.58
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	8	0.58
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	11	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	11	0.58
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	11	0.58
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	11	0.58
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	11	0.58
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	11	0.58
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	15	0.58
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	9	0.58
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	11	0.58
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	11	0.58
(1,353)	1:37:A:PRO:HA	1:40:A:ASN:H	4	0.58
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD11	10	0.58
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD12	10	0.58
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD13	10	0.58
(1,142)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	14	0.58
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	12	0.58
(1,64)	1:19:A:TRP:HA	1:22:A:PHE:H	8	0.58
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	14	0.58
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	4	0.58
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	1	0.57
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	1	0.57
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	1	0.57
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	2	0.57
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	2	0.57
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	2	0.57
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD22	7	0.57
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD23	7	0.57
(1,707)	1:66:A:MET:HB3	1:68:A:GLN:HB3	9	0.57
(1,707)	1:66:A:MET:HB3	1:68:A:GLN:HB2	9	0.57
(1,707)	1:66:A:MET:HB2	1:68:A:GLN:HB3	9	0.57
(1,707)	1:66:A:MET:HB2	1:68:A:GLN:HB2	9	0.57
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	14	0.57
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	3	0.57
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	3	0.57
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	3	0.57
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	3	0.57
(1,405)	1:42:A:MET:H	1:43:A:LEU:HG	4	0.57
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	8	0.57
(1,215)	1:27:A:LYS:HA	1:30:A:TYR:H	1	0.57
(1,210)	1:27:A:LYS:HD3	1:28:A:ASN:H	8	0.57
(1,210)	1:27:A:LYS:HD2	1:28:A:ASN:H	8	0.57
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	12	0.57
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	1	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	11	0.57
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	11	0.57
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	7	0.57
(1,1026)	1:103:A:VAL:H	1:104:A:LEU:HD21	11	0.56
(1,960)	1:97:A:ARG:HA	1:101:A:GLU:HB3	15	0.56
(1,960)	1:97:A:ARG:HA	1:101:A:GLU:HB2	15	0.56
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD22	5	0.56
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD23	5	0.56
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	6	0.56
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	6	0.56
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	9	0.56
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	1	0.56
(1,643)	1:60:A:GLU:H	1:61:A:LEU:HD21	7	0.56
(1,632)	1:59:A:GLU:HG2	1:104:A:LEU:HD21	2	0.56
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	14	0.56
(1,586)	1:58:A:VAL:HG13	1:61:A:LEU:HD21	7	0.56
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD22	6	0.56
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD23	6	0.56
(1,523)	1:53:A:THR:HA	1:57:A:ILE:H	13	0.56
(1,435)	1:46:A:ASP:HA	1:49:A:GLU:H	4	0.56
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	7	0.56
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	9	0.56
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	15	0.56
(1,329)	1:36:A:LEU:HD22	1:39:A:LEU:HD21	9	0.56
(1,329)	1:36:A:LEU:HD23	1:39:A:LEU:HD21	9	0.56
(1,210)	1:27:A:LYS:HD3	1:28:A:ASN:H	11	0.56
(1,210)	1:27:A:LYS:HD2	1:28:A:ASN:H	11	0.56
(1,201)	1:26:A:LEU:HG	1:30:A:TYR:H	3	0.56
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	14	0.56
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	14	0.56
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	6	0.56
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	11	0.56
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	12	0.56
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	4	0.56
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	4	0.55
(1,1020)	1:102:A:GLU:HA	1:105:A:LEU:H	10	0.55
(1,983)	1:100:A:LEU:HD22	1:102:A:GLU:H	12	0.55
(1,983)	1:100:A:LEU:HD23	1:102:A:GLU:H	12	0.55
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	3	0.55
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	3	0.55
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	3	0.55
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	1	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	1	0.55
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	11	0.55
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	3	0.55
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	4	0.55
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	4	0.55
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	2	0.55
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	2	0.55
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	10	0.55
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD22	11	0.55
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD23	11	0.55
(1,487)	1:51:A:LEU:HD21	1:54:A:ARG:H	13	0.55
(1,462)	1:50:A:ALA:HB1	1:51:A:LEU:HD21	4	0.55
(1,394)	1:40:A:ASN:H	1:41:A:LEU:HD22	14	0.55
(1,394)	1:40:A:ASN:H	1:41:A:LEU:HD23	14	0.55
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	1	0.55
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	5	0.55
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	7	0.55
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	7	0.55
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD11	14	0.55
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD12	14	0.55
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD13	14	0.55
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	2	0.55
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	5	0.55
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	5	0.55
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	15	0.55
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	15	0.55
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	3	0.55
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	11	0.55
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	6	0.54
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	6	0.54
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	6	0.54
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	9	0.54
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	9	0.54
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	9	0.54
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	7	0.54
(1,1067)	1:104:A:LEU:HA	1:106:A:LYS:H	10	0.54
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	8	0.54
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	15	0.54
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	14	0.54
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	1	0.54
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	1	0.54
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD11	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD12	4	0.54
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD13	4	0.54
(1,172)	1:25:A:LEU:HA	1:28:A:ASN:H	1	0.54
(1,960)	1:97:A:ARG:HA	1:101:A:GLU:HB3	8	0.53
(1,960)	1:97:A:ARG:HA	1:101:A:GLU:HB2	8	0.53
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	10	0.53
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	7	0.53
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	7	0.53
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	7	0.53
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	7	0.53
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	7	0.53
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	7	0.53
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	14	0.53
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	14	0.53
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	14	0.53
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	14	0.53
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	14	0.53
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	14	0.53
(1,850)	1:89:A:LEU:HD21	1:91:A:ALA:H	2	0.53
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	14	0.53
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	14	0.53
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	14	0.53
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	11	0.53
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	11	0.53
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	11	0.53
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	11	0.53
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	11	0.53
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	11	0.53
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	11	0.53
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	11	0.53
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	11	0.53
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	10	0.53
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	2	0.53
(1,676)	1:62:A:LEU:HD21	1:64:A:GLY:H	3	0.53
(1,663)	1:61:A:LEU:HD11	1:96:A:LEU:HD21	8	0.53
(1,663)	1:61:A:LEU:HD12	1:96:A:LEU:HD21	8	0.53
(1,663)	1:61:A:LEU:HD13	1:96:A:LEU:HD21	8	0.53
(1,598)	1:58:A:VAL:HG12	1:96:A:LEU:HD21	11	0.53
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	2	0.53
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	2	0.53
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	2	0.53
(1,353)	1:37:A:PRO:HA	1:40:A:ASN:H	15	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:36:A:LEU:HD11	1:39:A:LEU:HD21	10	0.53
(1,327)	1:36:A:LEU:HD12	1:39:A:LEU:HD21	10	0.53
(1,327)	1:36:A:LEU:HD13	1:39:A:LEU:HD21	10	0.53
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	11	0.53
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	8	0.53
(1,174)	1:25:A:LEU:HD11	1:28:A:ASN:HA	1	0.53
(1,174)	1:25:A:LEU:HD12	1:28:A:ASN:HA	1	0.53
(1,174)	1:25:A:LEU:HD13	1:28:A:ASN:HA	1	0.53
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	1	0.53
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	6	0.53
(1,71)	1:19:A:TRP:H	1:20:A:LEU:HD21	2	0.53
(1,66)	1:19:A:TRP:HA	1:23:A:VAL:H	13	0.53
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	1	0.53
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	6	0.52
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	6	0.52
(1,947)	1:96:A:LEU:HD23	1:100:A:LEU:HD21	1	0.52
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	10	0.52
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	3	0.52
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	6	0.52
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	6	0.52
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	6	0.52
(1,888)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	6	0.52
(1,888)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	6	0.52
(1,888)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	6	0.52
(1,860)	1:89:A:LEU:HD21	1:92:A:ALA:HB1	3	0.52
(1,822)	1:87:A:ASN:H	1:89:A:LEU:HD21	3	0.52
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	6	0.52
(1,563)	1:57:A:ILE:HG23	1:61:A:LEU:HD21	12	0.52
(1,282)	1:33:A:ASP:HA	1:36:A:LEU:HD11	11	0.52
(1,282)	1:33:A:ASP:HA	1:36:A:LEU:HD12	11	0.52
(1,282)	1:33:A:ASP:HA	1:36:A:LEU:HD13	11	0.52
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	5	0.52
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	7	0.52
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	2	0.51
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	2	0.51
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	2	0.51
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	10	0.51
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	10	0.51
(1,1012)	1:101:A:GLU:HA	1:105:A:LEU:HD22	6	0.51
(1,1012)	1:101:A:GLU:HA	1:105:A:LEU:HD23	6	0.51
(1,1011)	1:101:A:GLU:HA	1:105:A:LEU:HD21	10	0.51
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:93:A:PRO:HA	1:95:A:GLU:H	14	0.51
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	7	0.51
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	7	0.51
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	7	0.51
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	5	0.51
(1,675)	1:62:A:LEU:HD11	1:64:A:GLY:H	6	0.51
(1,675)	1:62:A:LEU:HD12	1:64:A:GLY:H	6	0.51
(1,675)	1:62:A:LEU:HD13	1:64:A:GLY:H	6	0.51
(1,590)	1:58:A:VAL:HG22	1:61:A:LEU:HD21	10	0.51
(1,564)	1:57:A:ILE:HG23	1:61:A:LEU:HD22	9	0.51
(1,564)	1:57:A:ILE:HG23	1:61:A:LEU:HD23	9	0.51
(1,559)	1:57:A:ILE:HG21	1:61:A:LEU:HD21	14	0.51
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	5	0.51
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	1	0.51
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	4	0.51
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	4	0.51
(1,223)	1:28:A:ASN:HA	1:32:A:ASN:H	8	0.51
(1,195)	1:26:A:LEU:HD21	1:29:A:ALA:HB1	9	0.51
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	1	0.51
(1,117)	1:22:A:PHE:HB3	1:25:A:LEU:HD21	15	0.51
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	8	0.51
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	8	0.51
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	9	0.51
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	9	0.51
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	10	0.51
(1,1022)	1:102:A:GLU:HA	1:106:A:LYS:H	7	0.5
(1,1012)	1:101:A:GLU:HA	1:105:A:LEU:HD22	11	0.5
(1,1012)	1:101:A:GLU:HA	1:105:A:LEU:HD23	11	0.5
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	5	0.5
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	8	0.5
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	8	0.5
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	8	0.5
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	14	0.5
(1,942)	1:96:A:LEU:HD21	1:100:A:LEU:HD21	9	0.5
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	4	0.5
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	2	0.5
(1,786)	1:78:A:GLY:H	1:81:A:THR:H	8	0.5
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	10	0.5
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	13	0.5
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	13	0.5
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG21	5	0.5
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG21	5	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG21	5	0.5
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG22	5	0.5
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG22	5	0.5
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG22	5	0.5
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG23	5	0.5
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG23	5	0.5
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG23	5	0.5
(1,546)	1:56:A:ARG:HG3	1:57:A:ILE:HA	5	0.5
(1,546)	1:56:A:ARG:HG2	1:57:A:ILE:HA	5	0.5
(1,486)	1:51:A:LEU:HD11	1:54:A:ARG:H	15	0.5
(1,486)	1:51:A:LEU:HD12	1:54:A:ARG:H	15	0.5
(1,486)	1:51:A:LEU:HD13	1:54:A:ARG:H	15	0.5
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	5	0.5
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	5	0.5
(1,402)	1:41:A:LEU:HG	1:42:A:MET:H	3	0.5
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	1	0.5
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	5	0.5
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	15	0.5
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	15	0.5
(1,181)	1:25:A:LEU:HD22	1:28:A:ASN:HB2	2	0.5
(1,181)	1:25:A:LEU:HD23	1:28:A:ASN:HB2	2	0.5
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	13	0.5
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	12	0.5
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	12	0.5
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	12	0.5
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	6	0.5
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	6	0.5
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	6	0.5
(1,80)	1:20:A:LEU:H	1:22:A:PHE:H	13	0.5
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	4	0.5
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	4	0.5
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	4	0.5
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	10	0.5
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD22	11	0.5
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD23	11	0.5
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	14	0.5
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	7	0.5
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	10	0.49
(1,1026)	1:103:A:VAL:H	1:104:A:LEU:HD21	10	0.49
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	11	0.49
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	14	0.49
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	10	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,693)	1:64:A:GLY:HA3	1:66:A:MET:HA	3	0.49
(1,693)	1:64:A:GLY:HA2	1:66:A:MET:HA	3	0.49
(1,644)	1:60:A:GLU:H	1:61:A:LEU:HD22	8	0.49
(1,644)	1:60:A:GLU:H	1:61:A:LEU:HD23	8	0.49
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	11	0.49
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	11	0.49
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	11	0.49
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	11	0.49
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG21	11	0.49
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG21	11	0.49
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG21	11	0.49
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG22	11	0.49
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG22	11	0.49
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG22	11	0.49
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG23	11	0.49
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG23	11	0.49
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG23	11	0.49
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	6	0.49
(1,509)	1:51:A:LEU:HD21	1:55:A:VAL:HG23	5	0.49
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	13	0.49
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	7	0.49
(1,400)	1:41:A:LEU:HD21	1:42:A:MET:H	6	0.49
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD11	4	0.49
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD12	4	0.49
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD13	4	0.49
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	12	0.49
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	12	0.49
(1,19)	1:15:A:ARG:HG3	1:19:A:TRP:H	5	0.49
(1,19)	1:15:A:ARG:HG2	1:19:A:TRP:H	5	0.49
(1,19)	1:15:A:ARG:HG3	1:19:A:TRP:H	6	0.49
(1,19)	1:15:A:ARG:HG2	1:19:A:TRP:H	6	0.49
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	15	0.48
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	15	0.48
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	4	0.48
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	10	0.48
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD22	4	0.48
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD23	4	0.48
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	14	0.48
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	15	0.48
(1,707)	1:66:A:MET:HB3	1:68:A:GLN:HB3	8	0.48
(1,707)	1:66:A:MET:HB3	1:68:A:GLN:HB2	8	0.48
(1,707)	1:66:A:MET:HB2	1:68:A:GLN:HB3	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,707)	1:66:A:MET:HB2	1:68:A:GLN:HB2	8	0.48
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	15	0.48
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	15	0.48
(1,598)	1:58:A:VAL:HG12	1:96:A:LEU:HD21	1	0.48
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	4	0.48
(1,546)	1:56:A:ARG:HG3	1:57:A:ILE:HA	3	0.48
(1,546)	1:56:A:ARG:HG2	1:57:A:ILE:HA	3	0.48
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	6	0.48
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	6	0.48
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	6	0.48
(1,420)	1:43:A:LEU:HD21	1:48:A:ARG:HD2	4	0.48
(1,353)	1:37:A:PRO:HA	1:40:A:ASN:H	13	0.48
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	3	0.48
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	1	0.48
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	4	0.48
(1,76)	1:20:A:LEU:HD21	1:21:A:ARG:H	12	0.48
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	14	0.47
(1,1026)	1:103:A:VAL:H	1:104:A:LEU:HD21	3	0.47
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	2	0.47
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	2	0.47
(1,827)	1:87:A:ASN:HA	1:89:A:LEU:HD21	3	0.47
(1,786)	1:78:A:GLY:H	1:81:A:THR:H	10	0.47
(1,786)	1:78:A:GLY:H	1:81:A:THR:H	14	0.47
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	12	0.47
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	12	0.47
(1,606)	1:58:A:VAL:HG23	1:96:A:LEU:HD21	3	0.47
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	15	0.47
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	15	0.47
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	15	0.47
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	15	0.47
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	15	0.47
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	15	0.47
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	6	0.47
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	6	0.47
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	6	0.47
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	6	0.47
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	6	0.47
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	11	0.47
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	11	0.47
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	11	0.47
(1,372)	1:38:A:LEU:HA	1:41:A:LEU:HD22	7	0.47
(1,372)	1:38:A:LEU:HA	1:41:A:LEU:HD23	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	10	0.47
(1,66)	1:19:A:TRP:HA	1:23:A:VAL:H	4	0.47
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	11	0.47
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	1	0.46
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	14	0.46
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	8	0.46
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	8	0.46
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	8	0.46
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	8	0.46
(1,639)	1:60:A:GLU:HA	1:63:A:ARG:HA	7	0.46
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	9	0.46
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	9	0.46
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	9	0.46
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	9	0.46
(1,600)	1:58:A:VAL:HG13	1:96:A:LEU:HD21	13	0.46
(1,509)	1:51:A:LEU:HD21	1:55:A:VAL:HG23	3	0.46
(1,497)	1:51:A:LEU:HA	1:55:A:VAL:H	15	0.46
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	15	0.46
(1,393)	1:40:A:ASN:H	1:41:A:LEU:HD21	15	0.46
(1,384)	1:39:A:LEU:HD21	1:40:A:ASN:H	7	0.46
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD22	9	0.46
(1,357)	1:37:A:PRO:HB3	1:41:A:LEU:HD23	9	0.46
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD11	9	0.46
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD12	9	0.46
(1,357)	1:37:A:PRO:HB2	1:41:A:LEU:HD13	9	0.46
(1,298)	1:35:A:HIS:HA	1:38:A:LEU:H	2	0.46
(1,248)	1:30:A:TYR:HE1	1:39:A:LEU:HD21	4	0.46
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	11	0.46
(1,114)	1:22:A:PHE:HA	1:25:A:LEU:H	1	0.46
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	1	0.46
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	15	0.45
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	15	0.45
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	15	0.45
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	5	0.45
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	5	0.45
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	5	0.45
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	5	0.45
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	5	0.45
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	5	0.45
(1,1026)	1:103:A:VAL:H	1:104:A:LEU:HD21	1	0.45
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	1	0.45
(1,983)	1:100:A:LEU:HD22	1:102:A:GLU:H	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,983)	1:100:A:LEU:HD23	1:102:A:GLU:H	7	0.45
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	11	0.45
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	11	0.45
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	15	0.45
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	15	0.45
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	11	0.45
(1,965)	1:98:A:GLN:HA	1:101:A:GLU:H	4	0.45
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD22	13	0.45
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD23	13	0.45
(1,933)	1:96:A:LEU:HD22	1:99:A:TRP:HB2	9	0.45
(1,933)	1:96:A:LEU:HD23	1:99:A:TRP:HB2	9	0.45
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	8	0.45
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	15	0.45
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	12	0.45
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	12	0.45
(1,786)	1:78:A:GLY:H	1:81:A:THR:H	12	0.45
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	2	0.45
(1,761)	1:72:A:LYS:HB3	1:76:A:GLY:H	14	0.45
(1,761)	1:72:A:LYS:HB2	1:76:A:GLY:H	14	0.45
(1,675)	1:62:A:LEU:HD11	1:64:A:GLY:H	1	0.45
(1,675)	1:62:A:LEU:HD12	1:64:A:GLY:H	1	0.45
(1,675)	1:62:A:LEU:HD13	1:64:A:GLY:H	1	0.45
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	3	0.45
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	9	0.45
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	14	0.45
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	2	0.45
(1,384)	1:39:A:LEU:HD21	1:40:A:ASN:H	11	0.45
(1,210)	1:27:A:LYS:HD3	1:28:A:ASN:H	6	0.45
(1,210)	1:27:A:LYS:HD2	1:28:A:ASN:H	6	0.45
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	3	0.45
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	3	0.45
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	1	0.45
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD22	10	0.45
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD23	10	0.45
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	9	0.45
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	12	0.45
(1,980)	1:100:A:LEU:HD22	1:101:A:GLU:H	7	0.44
(1,980)	1:100:A:LEU:HD23	1:101:A:GLU:H	7	0.44
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	4	0.44
(1,947)	1:96:A:LEU:HD23	1:100:A:LEU:HD21	7	0.44
(1,942)	1:96:A:LEU:HD21	1:100:A:LEU:HD21	14	0.44
(1,933)	1:96:A:LEU:HD22	1:99:A:TRP:HB2	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:96:A:LEU:HD23	1:99:A:TRP:HB2	8	0.44
(1,873)	1:90:A:LYS:HA	1:92:A:ALA:H	8	0.44
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	14	0.44
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	14	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	3	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	3	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	3	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	6	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	6	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	6	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	8	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	8	0.44
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	8	0.44
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	11	0.44
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	11	0.44
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	13	0.44
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	13	0.44
(1,632)	1:59:A:GLU:HG2	1:104:A:LEU:HD21	14	0.44
(1,586)	1:58:A:VAL:HG13	1:61:A:LEU:HD21	8	0.44
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	11	0.44
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	14	0.44
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	4	0.44
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD22	9	0.44
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD23	9	0.44
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD11	13	0.44
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD12	13	0.44
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD13	13	0.44
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD11	15	0.44
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD12	15	0.44
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD13	15	0.44
(1,329)	1:36:A:LEU:HD22	1:39:A:LEU:HD21	5	0.44
(1,329)	1:36:A:LEU:HD23	1:39:A:LEU:HD21	5	0.44
(1,223)	1:28:A:ASN:HA	1:32:A:ASN:H	9	0.44
(1,117)	1:22:A:PHE:HB3	1:25:A:LEU:HD21	12	0.44
(1,69)	1:19:A:TRP:H	1:20:A:LEU:HG	15	0.44
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	1	0.44
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	1	0.44
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	1	0.44
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	1	0.44
(1,13)	1:12:A:ALA:HA	1:15:A:ARG:H	1	0.44
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	5	0.43
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	14	0.43
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	14	0.43
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	12	0.43
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	12	0.43
(1,801)	1:81:A:THR:HA	1:84:A:ARG:H	3	0.43
(1,752)	1:71:A:LEU:HD11	1:74:A:GLU:HG3	1	0.43
(1,752)	1:71:A:LEU:HD12	1:74:A:GLU:HG3	1	0.43
(1,752)	1:71:A:LEU:HD13	1:74:A:GLU:HG3	1	0.43
(1,717)	1:67:A:SER:HA	1:70:A:GLU:H	8	0.43
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	4	0.43
(1,563)	1:57:A:ILE:HG23	1:61:A:LEU:HD21	13	0.43
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	5	0.43
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	3	0.43
(1,223)	1:28:A:ASN:HA	1:32:A:ASN:H	13	0.43
(1,201)	1:26:A:LEU:HG	1:30:A:TYR:H	5	0.43
(1,181)	1:25:A:LEU:HD22	1:28:A:ASN:HB2	9	0.43
(1,181)	1:25:A:LEU:HD23	1:28:A:ASN:HB2	9	0.43
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD22	3	0.43
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD23	3	0.43
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	7	0.43
(1,144)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	15	0.43
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	14	0.43
(1,31)	1:17:A:GLN:HA	1:19:A:TRP:H	5	0.43
(1,1076)	1:105:A:LEU:HD21	1:106:A:LYS:H	3	0.42
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	14	0.42
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	14	0.42
(1,1020)	1:102:A:GLU:HA	1:105:A:LEU:H	11	0.42
(1,972)	1:99:A:TRP:HA	1:102:A:GLU:H	4	0.42
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	14	0.42
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	14	0.42
(1,945)	1:96:A:LEU:HD22	1:100:A:LEU:HD21	11	0.42
(1,864)	1:89:A:LEU:HD21	1:92:A:ALA:HB3	15	0.42
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	13	0.42
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	4	0.42
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	4	0.42
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	9	0.42
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	9	0.42
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	9	0.42
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	10	0.42
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	10	0.42
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	10	0.42
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	14	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	14	0.42
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	15	0.42
(1,598)	1:58:A:VAL:HG12	1:96:A:LEU:HD21	9	0.42
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	3	0.42
(1,400)	1:41:A:LEU:HD21	1:42:A:MET:H	13	0.42
(1,384)	1:39:A:LEU:HD21	1:40:A:ASN:H	12	0.42
(1,353)	1:37:A:PRO:HA	1:40:A:ASN:H	7	0.42
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	11	0.42
(1,1052)	1:103:A:VAL:HA	1:106:A:LYS:H	12	0.41
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	15	0.41
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	15	0.41
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	15	0.41
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	13	0.41
(1,947)	1:96:A:LEU:HD23	1:100:A:LEU:HD21	5	0.41
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	6	0.41
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	11	0.41
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	10	0.41
(1,546)	1:56:A:ARG:HG3	1:57:A:ILE:HA	2	0.41
(1,546)	1:56:A:ARG:HG2	1:57:A:ILE:HA	2	0.41
(1,502)	1:51:A:LEU:HD22	1:55:A:VAL:HG12	7	0.41
(1,502)	1:51:A:LEU:HD23	1:55:A:VAL:HG12	7	0.41
(1,502)	1:51:A:LEU:HD11	1:55:A:VAL:HG13	7	0.41
(1,502)	1:51:A:LEU:HD12	1:55:A:VAL:HG13	7	0.41
(1,502)	1:51:A:LEU:HD13	1:55:A:VAL:HG13	7	0.41
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	13	0.41
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	13	0.41
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	13	0.41
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	13	0.41
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	13	0.41
(1,487)	1:51:A:LEU:HD21	1:54:A:ARG:H	5	0.41
(1,462)	1:50:A:ALA:HB1	1:51:A:LEU:HD21	10	0.41
(1,384)	1:39:A:LEU:HD21	1:40:A:ASN:H	13	0.41
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	6	0.41
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	6	0.41
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	9	0.41
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	9	0.41
(1,366)	1:38:A:LEU:HA	1:41:A:LEU:H	14	0.41
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD11	8	0.41
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD12	8	0.41
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD13	8	0.41
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	5	0.41
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:33:A:ASP:HA	1:35:A:HIS:HE1	15	0.41
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	11	0.41
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	15	0.41
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	13	0.41
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	13	0.41
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	13	0.41
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	8	0.41
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD22	13	0.41
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD23	13	0.41
(1,1076)	1:105:A:LEU:HD21	1:106:A:LYS:H	1	0.4
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	9	0.4
(1,1052)	1:103:A:VAL:HA	1:106:A:LYS:H	3	0.4
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	10	0.4
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	10	0.4
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	10	0.4
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	9	0.4
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	5	0.4
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	5	0.4
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	12	0.4
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	12	0.4
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	12	0.4
(1,722)	1:67:A:SER:HA	1:71:A:LEU:HD22	5	0.4
(1,722)	1:67:A:SER:HA	1:71:A:LEU:HD23	5	0.4
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	5	0.4
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	8	0.4
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	5	0.4
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	5	0.4
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	5	0.4
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	7	0.4
(1,372)	1:38:A:LEU:HA	1:41:A:LEU:HD22	11	0.4
(1,372)	1:38:A:LEU:HA	1:41:A:LEU:HD23	11	0.4
(1,333)	1:36:A:LEU:HD21	1:39:A:LEU:HD23	12	0.4
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD22	15	0.4
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD23	15	0.4
(1,201)	1:26:A:LEU:HG	1:30:A:TYR:H	2	0.4
(1,199)	1:26:A:LEU:HD21	1:29:A:ALA:HB3	11	0.4
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	5	0.4
(1,19)	1:15:A:ARG:HG3	1:19:A:TRP:H	8	0.4
(1,19)	1:15:A:ARG:HG2	1:19:A:TRP:H	8	0.4
(1,17)	1:15:A:ARG:HA	1:17:A:GLN:H	5	0.4
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	3	0.39
(1,1020)	1:102:A:GLU:HA	1:105:A:LEU:H	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:101:A:GLU:HA	1:105:A:LEU:HD22	9	0.39
(1,1012)	1:101:A:GLU:HA	1:105:A:LEU:HD23	9	0.39
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	9	0.39
(1,982)	1:100:A:LEU:HD21	1:102:A:GLU:H	1	0.39
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	7	0.39
(1,924)	1:96:A:LEU:HD22	1:98:A:GLN:H	1	0.39
(1,924)	1:96:A:LEU:HD23	1:98:A:GLN:H	1	0.39
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	5	0.39
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	5	0.39
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	7	0.39
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	7	0.39
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	10	0.39
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	10	0.39
(1,546)	1:56:A:ARG:HG3	1:57:A:ILE:HA	4	0.39
(1,546)	1:56:A:ARG:HG2	1:57:A:ILE:HA	4	0.39
(1,505)	1:51:A:LEU:HD21	1:55:A:VAL:HG21	3	0.39
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	8	0.39
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	8	0.39
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	8	0.39
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	8	0.39
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	8	0.39
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	2	0.39
(1,353)	1:37:A:PRO:HA	1:40:A:ASN:H	11	0.39
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	1	0.39
(1,172)	1:25:A:LEU:HA	1:28:A:ASN:H	2	0.39
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	5	0.39
(1,76)	1:20:A:LEU:HD21	1:21:A:ARG:H	9	0.39
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	7	0.39
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	14	0.38
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	2	0.38
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	12	0.38
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	2	0.38
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	2	0.38
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	2	0.38
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD22	7	0.38
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD23	7	0.38
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG11	5	0.38
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG12	5	0.38
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG13	5	0.38
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG21	5	0.38
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG22	5	0.38
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG23	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:89:A:LEU:HD21	1:92:A:ALA:HB2	4	0.38
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	1	0.38
(1,748)	1:71:A:LEU:HD21	1:72:A:LYS:H	5	0.38
(1,748)	1:71:A:LEU:HD21	1:72:A:LYS:H	12	0.38
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	15	0.38
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG3	9	0.38
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG2	9	0.38
(1,717)	1:67:A:SER:HA	1:70:A:GLU:H	4	0.38
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	4	0.38
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	14	0.38
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	14	0.38
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	14	0.38
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	14	0.38
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	14	0.38
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	14	0.38
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	7	0.38
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	13	0.38
(1,452)	1:48:A:ARG:HA	1:52:A:GLY:H	7	0.38
(1,435)	1:46:A:ASP:HA	1:49:A:GLU:H	5	0.38
(1,421)	1:43:A:LEU:HD22	1:48:A:ARG:HD2	8	0.38
(1,421)	1:43:A:LEU:HD23	1:48:A:ARG:HD2	8	0.38
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD11	5	0.38
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD12	5	0.38
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD13	5	0.38
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD22	13	0.38
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD23	13	0.38
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	6	0.38
(1,329)	1:36:A:LEU:HD22	1:39:A:LEU:HD21	6	0.38
(1,329)	1:36:A:LEU:HD23	1:39:A:LEU:HD21	6	0.38
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	8	0.38
(1,158)	1:24:A:ASP:HA	1:27:A:LYS:H	3	0.38
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	2	0.38
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	2	0.38
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	2	0.38
(1,103)	1:21:A:ARG:HA	1:24:A:ASP:H	3	0.38
(1,69)	1:19:A:TRP:H	1:20:A:LEU:HG	14	0.38
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	3	0.38
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	2	0.38
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	13	0.37
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	13	0.37
(1,945)	1:96:A:LEU:HD22	1:100:A:LEU:HD21	15	0.37
(1,864)	1:89:A:LEU:HD21	1:92:A:ALA:HB3	14	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	7	0.37
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	11	0.37
(1,693)	1:64:A:GLY:HA3	1:66:A:MET:HA	14	0.37
(1,693)	1:64:A:GLY:HA2	1:66:A:MET:HA	14	0.37
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD22	14	0.37
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD23	14	0.37
(1,563)	1:57:A:ILE:HG23	1:61:A:LEU:HD21	10	0.37
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	12	0.37
(1,471)	1:50:A:ALA:HB1	1:53:A:THR:HB	12	0.37
(1,471)	1:50:A:ALA:HB2	1:53:A:THR:HB	12	0.37
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD22	4	0.37
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD23	4	0.37
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD11	11	0.37
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD12	11	0.37
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD13	11	0.37
(1,278)	1:33:A:ASP:H	1:34:A:LEU:HG	12	0.37
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	9	0.37
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	6	0.37
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	9	0.37
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	13	0.37
(1,1070)	1:104:A:LEU:HD22	1:106:A:LYS:H	6	0.36
(1,1070)	1:104:A:LEU:HD23	1:106:A:LYS:H	6	0.36
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	12	0.36
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	12	0.36
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	4	0.36
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	4	0.36
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	4	0.36
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	4	0.36
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	4	0.36
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	4	0.36
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	9	0.36
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	9	0.36
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	9	0.36
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	9	0.36
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	9	0.36
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	9	0.36
(1,1022)	1:102:A:GLU:HA	1:106:A:LYS:H	3	0.36
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	14	0.36
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	14	0.36
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	14	0.36
(1,959)	1:97:A:ARG:HG3	1:101:A:GLU:H	8	0.36
(1,959)	1:97:A:ARG:HG2	1:101:A:GLU:H	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD22	1	0.36
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD23	1	0.36
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	6	0.36
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	5	0.36
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	6	0.36
(1,865)	1:89:A:LEU:HD22	1:92:A:ALA:HB3	10	0.36
(1,865)	1:89:A:LEU:HD23	1:92:A:ALA:HB3	10	0.36
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	3	0.36
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	10	0.36
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	14	0.36
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	9	0.36
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD11	13	0.36
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD12	13	0.36
(1,826)	1:87:A:ASN:HA	1:89:A:LEU:HD13	13	0.36
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	1	0.36
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	1	0.36
(1,797)	1:80:A:ALA:H	1:81:A:THR:HA	11	0.36
(1,748)	1:71:A:LEU:HD21	1:72:A:LYS:H	8	0.36
(1,693)	1:64:A:GLY:HA3	1:66:A:MET:HA	6	0.36
(1,693)	1:64:A:GLY:HA2	1:66:A:MET:HA	6	0.36
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	2	0.36
(1,492)	1:51:A:LEU:HD11	1:54:A:ARG:HD3	5	0.36
(1,492)	1:51:A:LEU:HD12	1:54:A:ARG:HD3	5	0.36
(1,492)	1:51:A:LEU:HD13	1:54:A:ARG:HD3	5	0.36
(1,441)	1:47:A:GLU:HA	1:49:A:GLU:H	14	0.36
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	11	0.36
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	11	0.36
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	15	0.36
(1,400)	1:41:A:LEU:HD21	1:42:A:MET:H	12	0.36
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	10	0.36
(1,384)	1:39:A:LEU:HD21	1:40:A:ASN:H	5	0.36
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD11	7	0.36
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD12	7	0.36
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD13	7	0.36
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	7	0.36
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	7	0.36
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	11	0.36
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	9	0.36
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	5	0.36
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	6	0.36
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	10	0.36
(1,933)	1:96:A:LEU:HD22	1:99:A:TRP:HB2	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:96:A:LEU:HD23	1:99:A:TRP:HB2	7	0.35
(1,864)	1:89:A:LEU:HD21	1:92:A:ALA:HB3	13	0.35
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	9	0.35
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	9	0.35
(1,693)	1:64:A:GLY:HA3	1:66:A:MET:HA	8	0.35
(1,693)	1:64:A:GLY:HA2	1:66:A:MET:HA	8	0.35
(1,563)	1:57:A:ILE:HG23	1:61:A:LEU:HD21	9	0.35
(1,523)	1:53:A:THR:HA	1:57:A:ILE:H	9	0.35
(1,502)	1:51:A:LEU:HD22	1:55:A:VAL:HG12	10	0.35
(1,502)	1:51:A:LEU:HD23	1:55:A:VAL:HG12	10	0.35
(1,502)	1:51:A:LEU:HD11	1:55:A:VAL:HG13	10	0.35
(1,502)	1:51:A:LEU:HD12	1:55:A:VAL:HG13	10	0.35
(1,502)	1:51:A:LEU:HD13	1:55:A:VAL:HG13	10	0.35
(1,492)	1:51:A:LEU:HD11	1:54:A:ARG:HD3	1	0.35
(1,492)	1:51:A:LEU:HD12	1:54:A:ARG:HD3	1	0.35
(1,492)	1:51:A:LEU:HD13	1:54:A:ARG:HD3	1	0.35
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	5	0.35
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	9	0.35
(1,384)	1:39:A:LEU:HD21	1:40:A:ASN:H	6	0.35
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	8	0.35
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	8	0.35
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	10	0.35
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	5	0.35
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	5	0.35
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	10	0.35
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	10	0.35
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	9	0.35
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB3	5	0.34
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB2	5	0.34
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	15	0.34
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	3	0.34
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	3	0.34
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	3	0.34
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	3	0.34
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	3	0.34
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	3	0.34
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	2	0.34
(1,983)	1:100:A:LEU:HD22	1:102:A:GLU:H	10	0.34
(1,983)	1:100:A:LEU:HD23	1:102:A:GLU:H	10	0.34
(1,980)	1:100:A:LEU:HD22	1:101:A:GLU:H	12	0.34
(1,980)	1:100:A:LEU:HD23	1:101:A:GLU:H	12	0.34
(1,972)	1:99:A:TRP:HA	1:102:A:GLU:H	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	12	0.34
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	12	0.34
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	11	0.34
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	13	0.34
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	11	0.34
(1,748)	1:71:A:LEU:HD21	1:72:A:LYS:H	13	0.34
(1,721)	1:67:A:SER:HA	1:71:A:LEU:HD21	7	0.34
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	2	0.34
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	9	0.34
(1,693)	1:64:A:GLY:HA3	1:66:A:MET:HA	7	0.34
(1,693)	1:64:A:GLY:HA2	1:66:A:MET:HA	7	0.34
(1,674)	1:62:A:LEU:HG	1:63:A:ARG:H	3	0.34
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	8	0.34
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	4	0.34
(1,559)	1:57:A:ILE:HG21	1:61:A:LEU:HD21	11	0.34
(1,546)	1:56:A:ARG:HG3	1:57:A:ILE:HA	6	0.34
(1,546)	1:56:A:ARG:HG2	1:57:A:ILE:HA	6	0.34
(1,546)	1:56:A:ARG:HG3	1:57:A:ILE:HA	8	0.34
(1,546)	1:56:A:ARG:HG2	1:57:A:ILE:HA	8	0.34
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	10	0.34
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	14	0.34
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	14	0.34
(1,353)	1:37:A:PRO:HA	1:40:A:ASN:H	14	0.34
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	13	0.34
(1,217)	1:27:A:LYS:HA	1:31:A:GLN:H	2	0.34
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	3	0.34
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	10	0.34
(1,197)	1:26:A:LEU:HD21	1:29:A:ALA:HB2	5	0.34
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	1	0.34
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	1	0.34
(1,69)	1:19:A:TRP:H	1:20:A:LEU:HG	7	0.34
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	7	0.34
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	8	0.34
(1,19)	1:15:A:ARG:HG3	1:19:A:TRP:H	4	0.34
(1,19)	1:15:A:ARG:HG2	1:19:A:TRP:H	4	0.34
(1,13)	1:12:A:ALA:HA	1:15:A:ARG:H	3	0.34
(1,13)	1:12:A:ALA:HA	1:15:A:ARG:H	6	0.34
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	12	0.33
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	12	0.33
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	12	0.33
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	12	0.33
(1,927)	1:96:A:LEU:HD21	1:99:A:TRP:H	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,897)	1:94:A:VAL:HA	1:95:A:GLU:H	8	0.33
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG11	14	0.33
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG12	14	0.33
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG13	14	0.33
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG21	14	0.33
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG22	14	0.33
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG23	14	0.33
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	8	0.33
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	7	0.33
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	7	0.33
(1,786)	1:78:A:GLY:H	1:81:A:THR:H	9	0.33
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	9	0.33
(1,632)	1:59:A:GLU:HG2	1:104:A:LEU:HD21	10	0.33
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	4	0.33
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	4	0.33
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	4	0.33
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	4	0.33
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	4	0.33
(1,492)	1:51:A:LEU:HD11	1:54:A:ARG:HD3	10	0.33
(1,492)	1:51:A:LEU:HD12	1:54:A:ARG:HD3	10	0.33
(1,492)	1:51:A:LEU:HD13	1:54:A:ARG:HD3	10	0.33
(1,480)	1:51:A:LEU:HD21	1:52:A:GLY:H	3	0.33
(1,437)	1:47:A:GLU:H	1:48:A:ARG:HB3	1	0.33
(1,437)	1:47:A:GLU:H	1:48:A:ARG:HB2	1	0.33
(1,400)	1:41:A:LEU:HD21	1:42:A:MET:H	1	0.33
(1,395)	1:40:A:ASN:HA	1:43:A:LEU:H	15	0.33
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	10	0.33
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	13	0.33
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	13	0.33
(1,351)	1:37:A:PRO:HG2	1:38:A:LEU:HD21	12	0.33
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD11	3	0.33
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD12	3	0.33
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD13	3	0.33
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD11	9	0.33
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD12	9	0.33
(1,348)	1:37:A:PRO:HG3	1:38:A:LEU:HD13	9	0.33
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	7	0.33
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	7	0.33
(1,278)	1:33:A:ASP:H	1:34:A:LEU:HG	15	0.33
(1,253)	1:31:A:GLN:H	1:33:A:ASP:H	10	0.33
(1,223)	1:28:A:ASN:HA	1:32:A:ASN:H	1	0.33
(1,103)	1:21:A:ARG:HA	1:24:A:ASP:H	14	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	3	0.33
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	3	0.33
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	4	0.33
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	4	0.33
(1,76)	1:20:A:LEU:HD21	1:21:A:ARG:H	6	0.33
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	14	0.33
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	4	0.33
(1,38)	1:17:A:GLN:HA	1:21:A:ARG:H	15	0.33
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	13	0.33
(1,19)	1:15:A:ARG:HG3	1:19:A:TRP:H	13	0.33
(1,19)	1:15:A:ARG:HG2	1:19:A:TRP:H	13	0.33
(1,1066)	1:104:A:LEU:H	1:106:A:LYS:H	4	0.32
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	11	0.32
(1,980)	1:100:A:LEU:HD22	1:101:A:GLU:H	13	0.32
(1,980)	1:100:A:LEU:HD23	1:101:A:GLU:H	13	0.32
(1,974)	1:99:A:TRP:HA	1:103:A:VAL:H	5	0.32
(1,965)	1:98:A:GLN:HA	1:101:A:GLU:H	13	0.32
(1,933)	1:96:A:LEU:HD22	1:99:A:TRP:HB2	2	0.32
(1,933)	1:96:A:LEU:HD23	1:99:A:TRP:HB2	2	0.32
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	6	0.32
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	6	0.32
(1,895)	1:93:A:PRO:HG3	1:97:A:ARG:H	10	0.32
(1,895)	1:93:A:PRO:HG2	1:97:A:ARG:H	10	0.32
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	15	0.32
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	8	0.32
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	12	0.32
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	12	0.32
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	12	0.32
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	12	0.32
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	12	0.32
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	12	0.32
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	12	0.32
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	12	0.32
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	12	0.32
(1,748)	1:71:A:LEU:HD21	1:72:A:LYS:H	4	0.32
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD22	5	0.32
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD23	5	0.32
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD22	15	0.32
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD23	15	0.32
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG3	7	0.32
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG2	7	0.32
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:51:A:LEU:HD11	1:54:A:ARG:H	5	0.32
(1,486)	1:51:A:LEU:HD12	1:54:A:ARG:H	5	0.32
(1,486)	1:51:A:LEU:HD13	1:54:A:ARG:H	5	0.32
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	8	0.32
(1,462)	1:50:A:ALA:HB1	1:51:A:LEU:HD21	13	0.32
(1,394)	1:40:A:ASN:H	1:41:A:LEU:HD22	15	0.32
(1,394)	1:40:A:ASN:H	1:41:A:LEU:HD23	15	0.32
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD11	3	0.32
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD12	3	0.32
(1,370)	1:38:A:LEU:HA	1:41:A:LEU:HD13	3	0.32
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	1	0.32
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	1	0.32
(1,248)	1:30:A:TYR:HE1	1:39:A:LEU:HD21	14	0.32
(1,215)	1:27:A:LYS:HA	1:30:A:TYR:H	13	0.32
(1,164)	1:24:A:ASP:H	1:25:A:LEU:HD21	2	0.32
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD11	8	0.32
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD12	8	0.32
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD13	8	0.32
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	5	0.32
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	6	0.32
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	11	0.32
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	14	0.32
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	14	0.32
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	12	0.32
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	12	0.32
(1,76)	1:20:A:LEU:HD21	1:21:A:ARG:H	2	0.32
(1,64)	1:19:A:TRP:HA	1:22:A:PHE:H	15	0.32
(1,62)	1:19:A:TRP:HZ2	1:20:A:LEU:HD22	6	0.32
(1,62)	1:19:A:TRP:HZ2	1:20:A:LEU:HD23	6	0.32
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	7	0.31
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	6	0.31
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	6	0.31
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	6	0.31
(1,980)	1:100:A:LEU:HD22	1:101:A:GLU:H	9	0.31
(1,980)	1:100:A:LEU:HD23	1:101:A:GLU:H	9	0.31
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	12	0.31
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	14	0.31
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	15	0.31
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	14	0.31
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	14	0.31
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	14	0.31
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	14	0.31
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	14	0.31
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	14	0.31
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	14	0.31
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	14	0.31
(1,779)	1:77:A:ALA:HB1	1:79:A:ILE:H	12	0.31
(1,779)	1:77:A:ALA:HB2	1:79:A:ILE:H	12	0.31
(1,779)	1:77:A:ALA:HB3	1:79:A:ILE:H	12	0.31
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	13	0.31
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	13	0.31
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	13	0.31
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	13	0.31
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	13	0.31
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	13	0.31
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	12	0.31
(1,693)	1:64:A:GLY:HA3	1:66:A:MET:HA	1	0.31
(1,693)	1:64:A:GLY:HA2	1:66:A:MET:HA	1	0.31
(1,607)	1:58:A:VAL:HG23	1:96:A:LEU:HD22	3	0.31
(1,607)	1:58:A:VAL:HG23	1:96:A:LEU:HD23	3	0.31
(1,546)	1:56:A:ARG:HG3	1:57:A:ILE:HA	1	0.31
(1,546)	1:56:A:ARG:HG2	1:57:A:ILE:HA	1	0.31
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	4	0.31
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	2	0.31
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	2	0.31
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	2	0.31
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	2	0.31
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	2	0.31
(1,468)	1:50:A:ALA:HA	1:53:A:THR:H	13	0.31
(1,459)	1:50:A:ALA:HA	1:51:A:LEU:H	12	0.31
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	14	0.31
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	14	0.31
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD22	7	0.31
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD23	7	0.31
(1,272)	1:32:A:ASN:HB2	1:34:A:LEU:HD21	3	0.31
(1,248)	1:30:A:TYR:HE1	1:39:A:LEU:HD21	3	0.31
(1,226)	1:29:A:ALA:HA	1:30:A:TYR:H	7	0.31
(1,181)	1:25:A:LEU:HD22	1:28:A:ASN:HB2	14	0.31
(1,181)	1:25:A:LEU:HD23	1:28:A:ASN:HB2	14	0.31
(1,172)	1:25:A:LEU:HA	1:28:A:ASN:H	5	0.31
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	13	0.31
(1,114)	1:22:A:PHE:HA	1:25:A:LEU:H	13	0.31
(1,107)	1:21:A:ARG:HB3	1:25:A:LEU:HD21	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	8	0.31
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD22	9	0.31
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD23	9	0.31
(1,64)	1:19:A:TRP:HA	1:22:A:PHE:H	14	0.31
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	15	0.31
(1,1083)	1:106:A:LYS:HG3	1:108:A:ASP:H	4	0.3
(1,1083)	1:106:A:LYS:HG2	1:108:A:ASP:H	4	0.3
(1,1070)	1:104:A:LEU:HD22	1:106:A:LYS:H	12	0.3
(1,1070)	1:104:A:LEU:HD23	1:106:A:LYS:H	12	0.3
(1,980)	1:100:A:LEU:HD22	1:101:A:GLU:H	8	0.3
(1,980)	1:100:A:LEU:HD23	1:101:A:GLU:H	8	0.3
(1,980)	1:100:A:LEU:HD22	1:101:A:GLU:H	10	0.3
(1,980)	1:100:A:LEU:HD23	1:101:A:GLU:H	10	0.3
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	9	0.3
(1,974)	1:99:A:TRP:HA	1:103:A:VAL:H	13	0.3
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	15	0.3
(1,959)	1:97:A:ARG:HG3	1:101:A:GLU:H	9	0.3
(1,959)	1:97:A:ARG:HG2	1:101:A:GLU:H	9	0.3
(1,945)	1:96:A:LEU:HD22	1:100:A:LEU:HD21	2	0.3
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD11	9	0.3
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD11	9	0.3
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD11	9	0.3
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD12	9	0.3
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD12	9	0.3
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD12	9	0.3
(1,780)	1:77:A:ALA:HB1	1:79:A:ILE:HD13	9	0.3
(1,780)	1:77:A:ALA:HB2	1:79:A:ILE:HD13	9	0.3
(1,780)	1:77:A:ALA:HB3	1:79:A:ILE:HD13	9	0.3
(1,717)	1:67:A:SER:HA	1:70:A:GLU:H	9	0.3
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	15	0.3
(1,480)	1:51:A:LEU:HD21	1:52:A:GLY:H	5	0.3
(1,435)	1:46:A:ASP:HA	1:49:A:GLU:H	12	0.3
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	7	0.3
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	7	0.3
(1,353)	1:37:A:PRO:HA	1:40:A:ASN:H	10	0.3
(1,166)	1:25:A:LEU:H	1:26:A:LEU:H	1	0.3
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD22	8	0.3
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD23	8	0.3
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	3	0.3
(1,103)	1:21:A:ARG:HA	1:24:A:ASP:H	13	0.3
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	9	0.3
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	10	0.3
(1,66)	1:19:A:TRP:HA	1:23:A:VAL:H	9	0.3
(1,1008)	1:101:A:GLU:HA	1:105:A:LEU:H	1	0.29
(1,965)	1:98:A:GLN:HA	1:101:A:GLU:H	2	0.29
(1,965)	1:98:A:GLN:HA	1:101:A:GLU:H	3	0.29
(1,933)	1:96:A:LEU:HD22	1:99:A:TRP:HB2	11	0.29
(1,933)	1:96:A:LEU:HD23	1:99:A:TRP:HB2	11	0.29
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG11	8	0.29
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG12	8	0.29
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG13	8	0.29
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG21	8	0.29
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG22	8	0.29
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG23	8	0.29
(1,864)	1:89:A:LEU:HD21	1:92:A:ALA:HB3	11	0.29
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	9	0.29
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	9	0.29
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	10	0.29
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	10	0.29
(1,755)	1:71:A:LEU:HD21	1:74:A:GLU:HG2	6	0.29
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG3	15	0.29
(1,728)	1:68:A:GLN:HA	1:72:A:LYS:HG2	15	0.29
(1,691)	1:64:A:GLY:H	1:66:A:MET:H	2	0.29
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG21	14	0.29
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG22	14	0.29
(1,547)	1:56:A:ARG:HG3	1:57:A:ILE:HG23	14	0.29
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG21	14	0.29
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG22	14	0.29
(1,547)	1:56:A:ARG:HG2	1:57:A:ILE:HG23	14	0.29
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	3	0.29
(1,298)	1:35:A:HIS:HA	1:38:A:LEU:H	6	0.29
(1,272)	1:32:A:ASN:HB2	1:34:A:LEU:HD21	2	0.29
(1,270)	1:32:A:ASN:HB3	1:34:A:LEU:HD21	3	0.29
(1,199)	1:26:A:LEU:HD21	1:29:A:ALA:HB3	15	0.29
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	7	0.29
(1,103)	1:21:A:ARG:HA	1:24:A:ASP:H	8	0.29
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	1	0.29
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	1	0.29
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	4	0.29
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	6	0.29
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	12	0.29
(1,1083)	1:106:A:LYS:HG3	1:108:A:ASP:H	1	0.28
(1,1083)	1:106:A:LYS:HG2	1:108:A:ASP:H	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	13	0.28
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	13	0.28
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	13	0.28
(1,1022)	1:102:A:GLU:HA	1:106:A:LYS:H	10	0.28
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	10	0.28
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	10	0.28
(1,965)	1:98:A:GLN:HA	1:101:A:GLU:H	6	0.28
(1,957)	1:97:A:ARG:HA	1:100:A:LEU:HD21	15	0.28
(1,860)	1:89:A:LEU:HD21	1:92:A:ALA:HB1	9	0.28
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	6	0.28
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	14	0.28
(1,824)	1:87:A:ASN:HA	1:88:A:SER:H	11	0.28
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	6	0.28
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	6	0.28
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	9	0.28
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	9	0.28
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	12	0.28
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	8	0.28
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	8	0.28
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	8	0.28
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	8	0.28
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	8	0.28
(1,623)	1:59:A:GLU:HA	1:104:A:LEU:HD22	11	0.28
(1,623)	1:59:A:GLU:HA	1:104:A:LEU:HD23	11	0.28
(1,563)	1:57:A:ILE:HG23	1:61:A:LEU:HD21	15	0.28
(1,546)	1:56:A:ARG:HG3	1:57:A:ILE:HA	7	0.28
(1,546)	1:56:A:ARG:HG2	1:57:A:ILE:HA	7	0.28
(1,546)	1:56:A:ARG:HG3	1:57:A:ILE:HA	10	0.28
(1,546)	1:56:A:ARG:HG2	1:57:A:ILE:HA	10	0.28
(1,441)	1:47:A:GLU:HA	1:49:A:GLU:H	8	0.28
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	10	0.28
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	10	0.28
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	1	0.28
(1,226)	1:29:A:ALA:HA	1:30:A:TYR:H	5	0.28
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	9	0.28
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	9	0.28
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD11	7	0.28
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD12	7	0.28
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD13	7	0.28
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	2	0.28
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	12	0.28
(1,117)	1:22:A:PHE:HB3	1:25:A:LEU:HD21	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:21:A:ARG:HB3	1:25:A:LEU:HD21	7	0.28
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	7	0.28
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	7	0.28
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	2	0.28
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	2	0.28
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	6	0.28
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	6	0.28
(1,76)	1:20:A:LEU:HD21	1:21:A:ARG:H	10	0.28
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD22	4	0.28
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD23	4	0.28
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD22	11	0.28
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD23	11	0.28
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	11	0.28
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	11	0.28
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	11	0.28
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	5	0.28
(1,19)	1:15:A:ARG:HG3	1:19:A:TRP:H	12	0.28
(1,19)	1:15:A:ARG:HG2	1:19:A:TRP:H	12	0.28
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB3	4	0.27
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB2	4	0.27
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	1	0.27
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	6	0.27
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	15	0.27
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	8	0.27
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	12	0.27
(1,945)	1:96:A:LEU:HD22	1:100:A:LEU:HD21	10	0.27
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	4	0.27
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	10	0.27
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	10	0.27
(1,739)	1:70:A:GLU:HG3	1:71:A:LEU:HD11	12	0.27
(1,739)	1:70:A:GLU:HG3	1:71:A:LEU:HD12	12	0.27
(1,739)	1:70:A:GLU:HG3	1:71:A:LEU:HD13	12	0.27
(1,707)	1:66:A:MET:HB3	1:68:A:GLN:HB3	7	0.27
(1,707)	1:66:A:MET:HB3	1:68:A:GLN:HB2	7	0.27
(1,707)	1:66:A:MET:HB2	1:68:A:GLN:HB3	7	0.27
(1,707)	1:66:A:MET:HB2	1:68:A:GLN:HB2	7	0.27
(1,638)	1:60:A:GLU:HA	1:63:A:ARG:H	13	0.27
(1,622)	1:59:A:GLU:HA	1:104:A:LEU:HD21	1	0.27
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	3	0.27
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	9	0.27
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	9	0.27
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	9	0.27
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	9	0.27
(1,486)	1:51:A:LEU:HD11	1:54:A:ARG:H	14	0.27
(1,486)	1:51:A:LEU:HD12	1:54:A:ARG:H	14	0.27
(1,486)	1:51:A:LEU:HD13	1:54:A:ARG:H	14	0.27
(1,459)	1:50:A:ALA:HA	1:51:A:LEU:H	6	0.27
(1,441)	1:47:A:GLU:HA	1:49:A:GLU:H	13	0.27
(1,441)	1:47:A:GLU:HA	1:49:A:GLU:H	15	0.27
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	15	0.27
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	15	0.27
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	15	0.27
(1,294)	1:35:A:HIS:HA	1:36:A:LEU:H	11	0.27
(1,217)	1:27:A:LYS:HA	1:31:A:GLN:H	8	0.27
(1,215)	1:27:A:LYS:HA	1:30:A:TYR:H	2	0.27
(1,210)	1:27:A:LYS:HD3	1:28:A:ASN:H	2	0.27
(1,210)	1:27:A:LYS:HD2	1:28:A:ASN:H	2	0.27
(1,172)	1:25:A:LEU:HA	1:28:A:ASN:H	7	0.27
(1,157)	1:24:A:ASP:HA	1:25:A:LEU:H	6	0.27
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	4	0.27
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	4	0.27
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	14	0.27
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	4	0.27
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	5	0.27
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	10	0.27
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	15	0.27
(1,1048)	1:103:A:VAL:HG23	1:104:A:LEU:HD21	13	0.26
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	13	0.26
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	4	0.26
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	4	0.26
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	4	0.26
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	6	0.26
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	1	0.26
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG11	3	0.26
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG12	3	0.26
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG13	3	0.26
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG21	3	0.26
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG22	3	0.26
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG23	3	0.26
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	7	0.26
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	7	0.26
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	1	0.26
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	12	0.26
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	1	0.26
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	4	0.26
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	4	0.26
(1,717)	1:67:A:SER:HA	1:70:A:GLU:H	5	0.26
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	3	0.26
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	15	0.26
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	15	0.26
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	15	0.26
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	15	0.26
(1,573)	1:58:A:VAL:HA	1:61:A:LEU:HG	12	0.26
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	12	0.26
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	12	0.26
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	12	0.26
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	12	0.26
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	12	0.26
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	12	0.26
(1,523)	1:53:A:THR:HA	1:57:A:ILE:H	12	0.26
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	5	0.26
(1,441)	1:47:A:GLU:HA	1:49:A:GLU:H	7	0.26
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	14	0.26
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	3	0.26
(1,384)	1:39:A:LEU:HD21	1:40:A:ASN:H	10	0.26
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	15	0.26
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	15	0.26
(1,298)	1:35:A:HIS:HA	1:38:A:LEU:H	12	0.26
(1,278)	1:33:A:ASP:H	1:34:A:LEU:HG	4	0.26
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	6	0.26
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	6	0.26
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	8	0.26
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	10	0.26
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	2	0.26
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	2	0.26
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	7	0.26
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	7	0.26
(1,75)	1:20:A:LEU:HD11	1:21:A:ARG:H	15	0.26
(1,75)	1:20:A:LEU:HD12	1:21:A:ARG:H	15	0.26
(1,75)	1:20:A:LEU:HD13	1:21:A:ARG:H	15	0.26
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	12	0.26
(1,19)	1:15:A:ARG:HG3	1:19:A:TRP:H	14	0.26
(1,19)	1:15:A:ARG:HG2	1:19:A:TRP:H	14	0.26
(1,1083)	1:106:A:LYS:HG3	1:108:A:ASP:H	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1083)	1:106:A:LYS:HG2	1:108:A:ASP:H	7	0.25
(1,1070)	1:104:A:LEU:HD22	1:106:A:LYS:H	11	0.25
(1,1070)	1:104:A:LEU:HD23	1:106:A:LYS:H	11	0.25
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	7	0.25
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	7	0.25
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	7	0.25
(1,1028)	1:103:A:VAL:HA	1:104:A:LEU:H	11	0.25
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	7	0.25
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	7	0.25
(1,965)	1:98:A:GLN:HA	1:101:A:GLU:H	14	0.25
(1,960)	1:97:A:ARG:HA	1:101:A:GLU:HB3	2	0.25
(1,960)	1:97:A:ARG:HA	1:101:A:GLU:HB2	2	0.25
(1,939)	1:96:A:LEU:HD13	1:100:A:LEU:HD21	1	0.25
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG11	13	0.25
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG12	13	0.25
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG13	13	0.25
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG21	13	0.25
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG22	13	0.25
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG23	13	0.25
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	6	0.25
(1,701)	1:65:A:GLU:H	1:66:A:MET:HA	1	0.25
(1,644)	1:60:A:GLU:H	1:61:A:LEU:HD22	1	0.25
(1,644)	1:60:A:GLU:H	1:61:A:LEU:HD23	1	0.25
(1,632)	1:59:A:GLU:HG2	1:104:A:LEU:HD21	7	0.25
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	4	0.25
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	4	0.25
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	4	0.25
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	4	0.25
(1,559)	1:57:A:ILE:HG21	1:61:A:LEU:HD21	1	0.25
(1,553)	1:57:A:ILE:HA	1:58:A:VAL:H	12	0.25
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	3	0.25
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	6	0.25
(1,447)	1:48:A:ARG:HA	1:49:A:GLU:H	5	0.25
(1,441)	1:47:A:GLU:HA	1:49:A:GLU:H	3	0.25
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	1	0.25
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	15	0.25
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	12	0.25
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	12	0.25
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	7	0.25
(1,328)	1:36:A:LEU:HD21	1:39:A:LEU:HD21	12	0.25
(1,191)	1:26:A:LEU:HA	1:29:A:ALA:H	5	0.25
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	2	0.25
(1,172)	1:25:A:LEU:HA	1:28:A:ASN:H	6	0.25
(1,161)	1:24:A:ASP:HA	1:28:A:ASN:H	4	0.25
(1,144)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	3	0.25
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	3	0.25
(1,99)	1:21:A:ARG:HA	1:22:A:PHE:H	13	0.25
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	12	0.25
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	12	0.25
(1,69)	1:19:A:TRP:H	1:20:A:LEU:HG	1	0.25
(1,64)	1:19:A:TRP:HA	1:22:A:PHE:H	10	0.25
(1,51)	1:18:A:GLU:HA	1:21:A:ARG:HD3	15	0.25
(1,51)	1:18:A:GLU:HA	1:21:A:ARG:HD2	15	0.25
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	2	0.25
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	1	0.25
(1,1083)	1:106:A:LYS:HG3	1:108:A:ASP:H	9	0.24
(1,1083)	1:106:A:LYS:HG2	1:108:A:ASP:H	9	0.24
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	7	0.24
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	3	0.24
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	3	0.24
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	3	0.24
(1,1004)	1:101:A:GLU:HA	1:102:A:GLU:H	3	0.24
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	5	0.24
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	5	0.24
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	11	0.24
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	9	0.24
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	9	0.24
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD11	2	0.24
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD12	2	0.24
(1,821)	1:87:A:ASN:H	1:89:A:LEU:HD13	2	0.24
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	4	0.24
(1,693)	1:64:A:GLY:HA3	1:66:A:MET:HA	9	0.24
(1,693)	1:64:A:GLY:HA2	1:66:A:MET:HA	9	0.24
(1,675)	1:62:A:LEU:HD11	1:64:A:GLY:H	2	0.24
(1,675)	1:62:A:LEU:HD12	1:64:A:GLY:H	2	0.24
(1,675)	1:62:A:LEU:HD13	1:64:A:GLY:H	2	0.24
(1,546)	1:56:A:ARG:HG3	1:57:A:ILE:HA	9	0.24
(1,546)	1:56:A:ARG:HG2	1:57:A:ILE:HA	9	0.24
(1,437)	1:47:A:GLU:H	1:48:A:ARG:HB3	7	0.24
(1,437)	1:47:A:GLU:H	1:48:A:ARG:HB2	7	0.24
(1,431)	1:46:A:ASP:HA	1:47:A:GLU:H	2	0.24
(1,394)	1:40:A:ASN:H	1:41:A:LEU:HD22	12	0.24
(1,394)	1:40:A:ASN:H	1:41:A:LEU:HD23	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	3	0.24
(1,384)	1:39:A:LEU:HD21	1:40:A:ASN:H	9	0.24
(1,298)	1:35:A:HIS:HA	1:38:A:LEU:H	1	0.24
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	8	0.24
(1,217)	1:27:A:LYS:HA	1:31:A:GLN:H	10	0.24
(1,191)	1:26:A:LEU:HA	1:29:A:ALA:H	4	0.24
(1,148)	1:23:A:VAL:HG22	1:26:A:LEU:HD21	15	0.24
(1,98)	1:21:A:ARG:H	1:22:A:PHE:H	11	0.24
(1,76)	1:20:A:LEU:HD21	1:21:A:ARG:H	11	0.24
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD22	2	0.24
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD23	2	0.24
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	4	0.24
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	11	0.23
(1,1026)	1:103:A:VAL:H	1:104:A:LEU:HD21	12	0.23
(1,980)	1:100:A:LEU:HD22	1:101:A:GLU:H	11	0.23
(1,980)	1:100:A:LEU:HD23	1:101:A:GLU:H	11	0.23
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	2	0.23
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	3	0.23
(1,848)	1:89:A:LEU:HA	1:91:A:ALA:H	8	0.23
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	2	0.23
(1,831)	1:88:A:SER:HA	1:89:A:LEU:H	6	0.23
(1,765)	1:74:A:GLU:H	1:76:A:GLY:H	8	0.23
(1,757)	1:72:A:LYS:HA	1:73:A:ASN:H	14	0.23
(1,748)	1:71:A:LEU:HD21	1:72:A:LYS:H	7	0.23
(1,740)	1:70:A:GLU:HG3	1:71:A:LEU:HD21	10	0.23
(1,717)	1:67:A:SER:HA	1:70:A:GLU:H	15	0.23
(1,695)	1:65:A:GLU:HA	1:66:A:MET:H	4	0.23
(1,675)	1:62:A:LEU:HD11	1:64:A:GLY:H	3	0.23
(1,675)	1:62:A:LEU:HD12	1:64:A:GLY:H	3	0.23
(1,675)	1:62:A:LEU:HD13	1:64:A:GLY:H	3	0.23
(1,586)	1:58:A:VAL:HG13	1:61:A:LEU:HD21	13	0.23
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	8	0.23
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG21	13	0.23
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG22	13	0.23
(1,548)	1:56:A:ARG:HD3	1:57:A:ILE:HG23	13	0.23
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG21	13	0.23
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG22	13	0.23
(1,548)	1:56:A:ARG:HD2	1:57:A:ILE:HG23	13	0.23
(1,535)	1:55:A:VAL:HA	1:56:A:ARG:H	3	0.23
(1,509)	1:51:A:LEU:HD21	1:55:A:VAL:HG23	1	0.23
(1,502)	1:51:A:LEU:HD22	1:55:A:VAL:HG12	14	0.23
(1,502)	1:51:A:LEU:HD23	1:55:A:VAL:HG12	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:51:A:LEU:HD11	1:55:A:VAL:HG13	14	0.23
(1,502)	1:51:A:LEU:HD12	1:55:A:VAL:HG13	14	0.23
(1,502)	1:51:A:LEU:HD13	1:55:A:VAL:HG13	14	0.23
(1,487)	1:51:A:LEU:HD21	1:54:A:ARG:H	4	0.23
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD11	9	0.23
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD12	9	0.23
(1,355)	1:37:A:PRO:HB3	1:41:A:LEU:HD13	9	0.23
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD11	12	0.23
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD12	12	0.23
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD13	12	0.23
(1,329)	1:36:A:LEU:HD22	1:39:A:LEU:HD21	7	0.23
(1,329)	1:36:A:LEU:HD23	1:39:A:LEU:HD21	7	0.23
(1,328)	1:36:A:LEU:HD21	1:39:A:LEU:HD21	8	0.23
(1,278)	1:33:A:ASP:H	1:34:A:LEU:HG	13	0.23
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD22	2	0.23
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD23	2	0.23
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	6	0.23
(1,201)	1:26:A:LEU:HG	1:30:A:TYR:H	1	0.23
(1,197)	1:26:A:LEU:HD21	1:29:A:ALA:HB2	15	0.23
(1,191)	1:26:A:LEU:HA	1:29:A:ALA:H	2	0.23
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD22	7	0.23
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD23	7	0.23
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	3	0.23
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	4	0.23
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	2	0.23
(1,76)	1:20:A:LEU:HD21	1:21:A:ARG:H	4	0.23
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	9	0.23
(1,19)	1:15:A:ARG:HG3	1:19:A:TRP:H	15	0.23
(1,19)	1:15:A:ARG:HG2	1:19:A:TRP:H	15	0.23
(1,13)	1:12:A:ALA:HA	1:15:A:ARG:H	7	0.23
(1,8)	1:11:A:MET:HA	1:12:A:ALA:H	5	0.23
(1,8)	1:11:A:MET:HA	1:12:A:ALA:H	12	0.23
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD11	14	0.22
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD11	14	0.22
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD12	14	0.22
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD12	14	0.22
(1,1060)	1:104:A:LEU:HB3	1:105:A:LEU:HD13	14	0.22
(1,1060)	1:104:A:LEU:HB2	1:105:A:LEU:HD13	14	0.22
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	9	0.22
(1,1026)	1:103:A:VAL:H	1:104:A:LEU:HD21	4	0.22
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	6	0.22
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,960)	1:97:A:ARG:HA	1:101:A:GLU:HB3	9	0.22
(1,960)	1:97:A:ARG:HA	1:101:A:GLU:HB2	9	0.22
(1,924)	1:96:A:LEU:HD22	1:98:A:GLN:H	15	0.22
(1,924)	1:96:A:LEU:HD23	1:98:A:GLN:H	15	0.22
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG3	15	0.22
(1,913)	1:95:A:GLU:H	1:98:A:GLN:HG2	15	0.22
(1,897)	1:94:A:VAL:HA	1:95:A:GLU:H	5	0.22
(1,895)	1:93:A:PRO:HG3	1:97:A:ARG:H	14	0.22
(1,895)	1:93:A:PRO:HG2	1:97:A:ARG:H	14	0.22
(1,875)	1:91:A:ALA:HA	1:92:A:ALA:H	10	0.22
(1,860)	1:89:A:LEU:HD21	1:92:A:ALA:HB1	7	0.22
(1,855)	1:89:A:LEU:HG	1:92:A:ALA:H	12	0.22
(1,853)	1:89:A:LEU:HA	1:92:A:ALA:H	6	0.22
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	10	0.22
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	6	0.22
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	6	0.22
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	15	0.22
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	15	0.22
(1,824)	1:87:A:ASN:HA	1:88:A:SER:H	15	0.22
(1,801)	1:81:A:THR:HA	1:84:A:ARG:H	1	0.22
(1,786)	1:78:A:GLY:H	1:81:A:THR:H	4	0.22
(1,632)	1:59:A:GLU:HG2	1:104:A:LEU:HD21	5	0.22
(1,604)	1:58:A:VAL:HG22	1:96:A:LEU:HD21	13	0.22
(1,588)	1:58:A:VAL:HG21	1:61:A:LEU:HD21	14	0.22
(1,559)	1:57:A:ILE:HG21	1:61:A:LEU:HD21	5	0.22
(1,523)	1:53:A:THR:HA	1:57:A:ILE:H	11	0.22
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	1	0.22
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	1	0.22
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	1	0.22
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	1	0.22
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	1	0.22
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	12	0.22
(1,468)	1:50:A:ALA:HA	1:53:A:THR:H	15	0.22
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD22	11	0.22
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD23	11	0.22
(1,333)	1:36:A:LEU:HD21	1:39:A:LEU:HD23	6	0.22
(1,266)	1:32:A:ASN:HA	1:34:A:LEU:HD21	8	0.22
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	14	0.22
(1,84)	1:20:A:LEU:HD11	1:23:A:VAL:HG11	1	0.22
(1,84)	1:20:A:LEU:HD12	1:23:A:VAL:HG11	1	0.22
(1,84)	1:20:A:LEU:HD13	1:23:A:VAL:HG11	1	0.22
(1,66)	1:19:A:TRP:HA	1:23:A:VAL:H	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:19:A:TRP:HA	1:22:A:PHE:H	13	0.22
(1,1062)	1:104:A:LEU:HB3	1:105:A:LEU:HD22	11	0.21
(1,1062)	1:104:A:LEU:HB2	1:105:A:LEU:HD22	11	0.21
(1,1062)	1:104:A:LEU:HB3	1:105:A:LEU:HD23	11	0.21
(1,1062)	1:104:A:LEU:HB2	1:105:A:LEU:HD23	11	0.21
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	11	0.21
(1,979)	1:100:A:LEU:HD21	1:101:A:GLU:H	12	0.21
(1,976)	1:100:A:LEU:HA	1:101:A:GLU:H	15	0.21
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	7	0.21
(1,935)	1:96:A:LEU:HD11	1:100:A:LEU:HD21	10	0.21
(1,930)	1:96:A:LEU:HD21	1:99:A:TRP:HB3	6	0.21
(1,856)	1:89:A:LEU:HD11	1:92:A:ALA:H	1	0.21
(1,856)	1:89:A:LEU:HD12	1:92:A:ALA:H	1	0.21
(1,856)	1:89:A:LEU:HD13	1:92:A:ALA:H	1	0.21
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	12	0.21
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	13	0.21
(1,719)	1:67:A:SER:HA	1:71:A:LEU:H	6	0.21
(1,695)	1:65:A:GLU:HA	1:66:A:MET:H	2	0.21
(1,675)	1:62:A:LEU:HD11	1:64:A:GLY:H	5	0.21
(1,675)	1:62:A:LEU:HD12	1:64:A:GLY:H	5	0.21
(1,675)	1:62:A:LEU:HD13	1:64:A:GLY:H	5	0.21
(1,668)	1:61:A:LEU:HD22	1:96:A:LEU:HD22	4	0.21
(1,668)	1:61:A:LEU:HD23	1:96:A:LEU:HD22	4	0.21
(1,668)	1:61:A:LEU:HD11	1:96:A:LEU:HD23	4	0.21
(1,668)	1:61:A:LEU:HD12	1:96:A:LEU:HD23	4	0.21
(1,668)	1:61:A:LEU:HD13	1:96:A:LEU:HD23	4	0.21
(1,625)	1:59:A:GLU:HB3	1:104:A:LEU:HD21	6	0.21
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	12	0.21
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	12	0.21
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	12	0.21
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	12	0.21
(1,586)	1:58:A:VAL:HG13	1:61:A:LEU:HD21	9	0.21
(1,553)	1:57:A:ILE:HA	1:58:A:VAL:H	8	0.21
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	9	0.21
(1,497)	1:51:A:LEU:HA	1:55:A:VAL:H	13	0.21
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	11	0.21
(1,421)	1:43:A:LEU:HD22	1:48:A:ARG:HD2	12	0.21
(1,421)	1:43:A:LEU:HD23	1:48:A:ARG:HD2	12	0.21
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD22	10	0.21
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD23	10	0.21
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD22	9	0.21
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD23	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:28:A:ASN:HA	1:32:A:ASN:H	10	0.21
(1,201)	1:26:A:LEU:HG	1:30:A:TYR:H	9	0.21
(1,174)	1:25:A:LEU:HD11	1:28:A:ASN:HA	15	0.21
(1,174)	1:25:A:LEU:HD12	1:28:A:ASN:HA	15	0.21
(1,174)	1:25:A:LEU:HD13	1:28:A:ASN:HA	15	0.21
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	13	0.21
(1,98)	1:21:A:ARG:H	1:22:A:PHE:H	9	0.21
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	11	0.21
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	11	0.21
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	9	0.21
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	14	0.21
(1,38)	1:17:A:GLN:HA	1:21:A:ARG:H	3	0.21
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	12	0.2
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	12	0.2
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	12	0.2
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	13	0.2
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	14	0.2
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	9	0.2
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	9	0.2
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	9	0.2
(1,968)	1:99:A:TRP:HA	1:100:A:LEU:H	4	0.2
(1,966)	1:98:A:GLN:HA	1:102:A:GLU:H	1	0.2
(1,932)	1:96:A:LEU:HD21	1:99:A:TRP:HB2	3	0.2
(1,892)	1:93:A:PRO:HG3	1:94:A:VAL:H	10	0.2
(1,892)	1:93:A:PRO:HG2	1:94:A:VAL:H	10	0.2
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	3	0.2
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	3	0.2
(1,748)	1:71:A:LEU:HD21	1:72:A:LYS:H	9	0.2
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	14	0.2
(1,717)	1:67:A:SER:HA	1:70:A:GLU:H	10	0.2
(1,638)	1:60:A:GLU:HA	1:63:A:ARG:H	15	0.2
(1,492)	1:51:A:LEU:HD11	1:54:A:ARG:HD3	4	0.2
(1,492)	1:51:A:LEU:HD12	1:54:A:ARG:HD3	4	0.2
(1,492)	1:51:A:LEU:HD13	1:54:A:ARG:HD3	4	0.2
(1,486)	1:51:A:LEU:HD11	1:54:A:ARG:H	7	0.2
(1,486)	1:51:A:LEU:HD12	1:54:A:ARG:H	7	0.2
(1,486)	1:51:A:LEU:HD13	1:54:A:ARG:H	7	0.2
(1,441)	1:47:A:GLU:HA	1:49:A:GLU:H	9	0.2
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	2	0.2
(1,405)	1:42:A:MET:H	1:43:A:LEU:HG	6	0.2
(1,388)	1:39:A:LEU:HA	1:43:A:LEU:H	12	0.2
(1,366)	1:38:A:LEU:HA	1:41:A:LEU:H	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD22	14	0.2
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD23	14	0.2
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	11	0.2
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	11	0.2
(1,264)	1:32:A:ASN:H	1:34:A:LEU:HG	10	0.2
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	8	0.2
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	8	0.2
(1,182)	1:25:A:LEU:HA	1:29:A:ALA:H	10	0.2
(1,180)	1:25:A:LEU:HD21	1:28:A:ASN:HB2	3	0.2
(1,174)	1:25:A:LEU:HD11	1:28:A:ASN:HA	8	0.2
(1,174)	1:25:A:LEU:HD12	1:28:A:ASN:HA	8	0.2
(1,174)	1:25:A:LEU:HD13	1:28:A:ASN:HA	8	0.2
(1,172)	1:25:A:LEU:HA	1:28:A:ASN:H	9	0.2
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD11	13	0.2
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD12	13	0.2
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD13	13	0.2
(1,158)	1:24:A:ASP:HA	1:27:A:LYS:H	10	0.2
(1,157)	1:24:A:ASP:HA	1:25:A:LEU:H	5	0.2
(1,157)	1:24:A:ASP:HA	1:25:A:LEU:H	11	0.2
(1,144)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	14	0.2
(1,137)	1:23:A:VAL:HB	1:26:A:LEU:HD21	7	0.2
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	7	0.2
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	6	0.2
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	15	0.2
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	12	0.2
(1,10)	1:12:A:ALA:HA	1:13:A:GLU:H	15	0.2
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB3	2	0.19
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB2	2	0.19
(1,1070)	1:104:A:LEU:HD22	1:106:A:LYS:H	8	0.19
(1,1070)	1:104:A:LEU:HD23	1:106:A:LYS:H	8	0.19
(1,1070)	1:104:A:LEU:HD22	1:106:A:LYS:H	13	0.19
(1,1070)	1:104:A:LEU:HD23	1:106:A:LYS:H	13	0.19
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	8	0.19
(1,983)	1:100:A:LEU:HD22	1:102:A:GLU:H	9	0.19
(1,983)	1:100:A:LEU:HD23	1:102:A:GLU:H	9	0.19
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	5	0.19
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	5	0.19
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	5	0.19
(1,959)	1:97:A:ARG:HG3	1:101:A:GLU:H	15	0.19
(1,959)	1:97:A:ARG:HG2	1:101:A:GLU:H	15	0.19
(1,947)	1:96:A:LEU:HD23	1:100:A:LEU:HD21	15	0.19
(1,945)	1:96:A:LEU:HD22	1:100:A:LEU:HD21	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:96:A:LEU:HD21	1:100:A:LEU:HD21	11	0.19
(1,909)	1:95:A:GLU:HA	1:96:A:LEU:H	14	0.19
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	15	0.19
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	15	0.19
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD22	15	0.19
(1,823)	1:87:A:ASN:H	1:89:A:LEU:HD23	15	0.19
(1,650)	1:61:A:LEU:HA	1:64:A:GLY:H	14	0.19
(1,649)	1:61:A:LEU:HA	1:62:A:LEU:H	8	0.19
(1,553)	1:57:A:ILE:HA	1:58:A:VAL:H	2	0.19
(1,553)	1:57:A:ILE:HA	1:58:A:VAL:H	4	0.19
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	10	0.19
(1,535)	1:55:A:VAL:HA	1:56:A:ARG:H	1	0.19
(1,486)	1:51:A:LEU:HD11	1:54:A:ARG:H	6	0.19
(1,486)	1:51:A:LEU:HD12	1:54:A:ARG:H	6	0.19
(1,486)	1:51:A:LEU:HD13	1:54:A:ARG:H	6	0.19
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	10	0.19
(1,454)	1:49:A:GLU:HA	1:50:A:ALA:H	10	0.19
(1,443)	1:47:A:GLU:HA	1:50:A:ALA:H	12	0.19
(1,398)	1:41:A:LEU:HA	1:42:A:MET:H	9	0.19
(1,398)	1:41:A:LEU:HA	1:42:A:MET:H	10	0.19
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD11	10	0.19
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD12	10	0.19
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD13	10	0.19
(1,320)	1:36:A:LEU:HD11	1:39:A:LEU:HD11	9	0.19
(1,320)	1:36:A:LEU:HD12	1:39:A:LEU:HD11	9	0.19
(1,320)	1:36:A:LEU:HD13	1:39:A:LEU:HD11	9	0.19
(1,298)	1:35:A:HIS:HA	1:38:A:LEU:H	11	0.19
(1,297)	1:35:A:HIS:HE1	1:36:A:LEU:H	3	0.19
(1,221)	1:28:A:ASN:HA	1:31:A:GLN:H	11	0.19
(1,206)	1:27:A:LYS:HA	1:28:A:ASN:H	4	0.19
(1,167)	1:25:A:LEU:HA	1:26:A:LEU:H	10	0.19
(1,166)	1:25:A:LEU:H	1:26:A:LEU:H	11	0.19
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD22	14	0.19
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD23	14	0.19
(1,99)	1:21:A:ARG:HA	1:22:A:PHE:H	4	0.19
(1,80)	1:20:A:LEU:H	1:22:A:PHE:H	15	0.19
(1,78)	1:20:A:LEU:HA	1:21:A:ARG:H	6	0.19
(1,76)	1:20:A:LEU:HD21	1:21:A:ARG:H	13	0.19
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD22	7	0.19
(1,72)	1:19:A:TRP:H	1:20:A:LEU:HD23	7	0.19
(1,69)	1:19:A:TRP:H	1:20:A:LEU:HG	4	0.19
(1,66)	1:19:A:TRP:HA	1:23:A:VAL:H	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	7	0.19
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD22	9	0.19
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD23	9	0.19
(1,32)	1:17:A:GLN:HA	1:20:A:LEU:H	10	0.19
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	3	0.19
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	14	0.19
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB3	8	0.18
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB2	8	0.18
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	10	0.18
(1,1008)	1:101:A:GLU:HA	1:105:A:LEU:H	5	0.18
(1,980)	1:100:A:LEU:HD22	1:101:A:GLU:H	15	0.18
(1,980)	1:100:A:LEU:HD23	1:101:A:GLU:H	15	0.18
(1,974)	1:99:A:TRP:HA	1:103:A:VAL:H	7	0.18
(1,965)	1:98:A:GLN:HA	1:101:A:GLU:H	10	0.18
(1,898)	1:94:A:VAL:HB	1:95:A:GLU:H	7	0.18
(1,892)	1:93:A:PRO:HG3	1:94:A:VAL:H	1	0.18
(1,892)	1:93:A:PRO:HG2	1:94:A:VAL:H	1	0.18
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	4	0.18
(1,844)	1:89:A:LEU:HA	1:90:A:LYS:HA	5	0.18
(1,762)	1:73:A:ASN:HA	1:74:A:GLU:H	3	0.18
(1,762)	1:73:A:ASN:HA	1:74:A:GLU:H	8	0.18
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD22	13	0.18
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD23	13	0.18
(1,738)	1:70:A:GLU:HG3	1:71:A:LEU:HB3	11	0.18
(1,738)	1:70:A:GLU:HG3	1:71:A:LEU:HB2	11	0.18
(1,738)	1:70:A:GLU:HG2	1:71:A:LEU:HB3	11	0.18
(1,738)	1:70:A:GLU:HG2	1:71:A:LEU:HB2	11	0.18
(1,623)	1:59:A:GLU:HA	1:104:A:LEU:HD22	5	0.18
(1,623)	1:59:A:GLU:HA	1:104:A:LEU:HD23	5	0.18
(1,596)	1:58:A:VAL:HG11	1:96:A:LEU:HD21	14	0.18
(1,584)	1:58:A:VAL:HG12	1:61:A:LEU:HD21	3	0.18
(1,480)	1:51:A:LEU:HD21	1:52:A:GLY:H	2	0.18
(1,454)	1:49:A:GLU:HA	1:50:A:ALA:H	1	0.18
(1,418)	1:43:A:LEU:HD21	1:48:A:ARG:HD3	4	0.18
(1,386)	1:39:A:LEU:HA	1:42:A:MET:H	9	0.18
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	9	0.18
(1,282)	1:33:A:ASP:HA	1:36:A:LEU:HD11	3	0.18
(1,282)	1:33:A:ASP:HA	1:36:A:LEU:HD12	3	0.18
(1,282)	1:33:A:ASP:HA	1:36:A:LEU:HD13	3	0.18
(1,278)	1:33:A:ASP:H	1:34:A:LEU:HG	14	0.18
(1,243)	1:30:A:TYR:HA	1:31:A:GLN:H	9	0.18
(1,191)	1:26:A:LEU:HA	1:29:A:ALA:H	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:26:A:LEU:HA	1:29:A:ALA:H	12	0.18
(1,167)	1:25:A:LEU:HA	1:26:A:LEU:H	1	0.18
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD22	15	0.18
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD23	15	0.18
(1,158)	1:24:A:ASP:HA	1:27:A:LYS:H	9	0.18
(1,155)	1:24:A:ASP:HA	1:25:A:LEU:HA	8	0.18
(1,144)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	1	0.18
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	3	0.18
(1,114)	1:22:A:PHE:HA	1:25:A:LEU:H	6	0.18
(1,107)	1:21:A:ARG:HB3	1:25:A:LEU:HD21	12	0.18
(1,98)	1:21:A:ARG:H	1:22:A:PHE:H	6	0.18
(1,84)	1:20:A:LEU:HD11	1:23:A:VAL:HG11	7	0.18
(1,84)	1:20:A:LEU:HD12	1:23:A:VAL:HG11	7	0.18
(1,84)	1:20:A:LEU:HD13	1:23:A:VAL:HG11	7	0.18
(1,64)	1:19:A:TRP:HA	1:22:A:PHE:H	4	0.18
(1,38)	1:17:A:GLN:HA	1:21:A:ARG:H	8	0.18
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD22	14	0.18
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD23	14	0.18
(1,35)	1:17:A:GLN:HA	1:20:A:LEU:HD21	14	0.18
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	7	0.18
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	8	0.18
(1,13)	1:12:A:ALA:HA	1:15:A:ARG:H	4	0.18
(1,1028)	1:103:A:VAL:HA	1:104:A:LEU:H	12	0.17
(1,1018)	1:102:A:GLU:H	1:104:A:LEU:H	6	0.17
(1,1014)	1:102:A:GLU:HA	1:103:A:VAL:H	14	0.17
(1,1008)	1:101:A:GLU:HA	1:105:A:LEU:H	9	0.17
(1,1008)	1:101:A:GLU:HA	1:105:A:LEU:H	11	0.17
(1,976)	1:100:A:LEU:HA	1:101:A:GLU:H	1	0.17
(1,942)	1:96:A:LEU:HD21	1:100:A:LEU:HD21	1	0.17
(1,831)	1:88:A:SER:HA	1:89:A:LEU:H	2	0.17
(1,831)	1:88:A:SER:HA	1:89:A:LEU:H	10	0.17
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD22	10	0.17
(1,828)	1:87:A:ASN:HA	1:89:A:LEU:HD23	10	0.17
(1,824)	1:87:A:ASN:HA	1:88:A:SER:H	4	0.17
(1,738)	1:70:A:GLU:HG3	1:71:A:LEU:HB3	12	0.17
(1,738)	1:70:A:GLU:HG3	1:71:A:LEU:HB2	12	0.17
(1,738)	1:70:A:GLU:HG2	1:71:A:LEU:HB3	12	0.17
(1,738)	1:70:A:GLU:HG2	1:71:A:LEU:HB2	12	0.17
(1,722)	1:67:A:SER:HA	1:71:A:LEU:HD22	7	0.17
(1,722)	1:67:A:SER:HA	1:71:A:LEU:HD23	7	0.17
(1,674)	1:62:A:LEU:HG	1:63:A:ARG:H	1	0.17
(1,649)	1:61:A:LEU:HA	1:62:A:LEU:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG21	4	0.17
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG21	4	0.17
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG21	4	0.17
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG22	4	0.17
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG22	4	0.17
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG22	4	0.17
(1,565)	1:57:A:ILE:HG21	1:81:A:THR:HG23	4	0.17
(1,565)	1:57:A:ILE:HG22	1:81:A:THR:HG23	4	0.17
(1,565)	1:57:A:ILE:HG23	1:81:A:THR:HG23	4	0.17
(1,535)	1:55:A:VAL:HA	1:56:A:ARG:H	2	0.17
(1,533)	1:54:A:ARG:HA	1:58:A:VAL:H	14	0.17
(1,491)	1:51:A:LEU:HD22	1:54:A:ARG:HA	1	0.17
(1,491)	1:51:A:LEU:HD23	1:54:A:ARG:HA	1	0.17
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	11	0.17
(1,486)	1:51:A:LEU:HD11	1:54:A:ARG:H	4	0.17
(1,486)	1:51:A:LEU:HD12	1:54:A:ARG:H	4	0.17
(1,486)	1:51:A:LEU:HD13	1:54:A:ARG:H	4	0.17
(1,459)	1:50:A:ALA:HA	1:51:A:LEU:H	11	0.17
(1,459)	1:50:A:ALA:HA	1:51:A:LEU:H	14	0.17
(1,454)	1:49:A:GLU:HA	1:50:A:ALA:H	14	0.17
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	6	0.17
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	6	0.17
(1,406)	1:42:A:MET:HA	1:43:A:LEU:H	12	0.17
(1,394)	1:40:A:ASN:H	1:41:A:LEU:HD22	6	0.17
(1,394)	1:40:A:ASN:H	1:41:A:LEU:HD23	6	0.17
(1,390)	1:40:A:ASN:HA	1:41:A:LEU:H	12	0.17
(1,372)	1:38:A:LEU:HA	1:41:A:LEU:HD22	6	0.17
(1,372)	1:38:A:LEU:HA	1:41:A:LEU:HD23	6	0.17
(1,353)	1:37:A:PRO:HA	1:40:A:ASN:H	9	0.17
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	13	0.17
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	13	0.17
(1,333)	1:36:A:LEU:HD21	1:39:A:LEU:HD23	9	0.17
(1,294)	1:35:A:HIS:HA	1:36:A:LEU:H	14	0.17
(1,172)	1:25:A:LEU:HA	1:28:A:ASN:H	10	0.17
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD22	4	0.17
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD23	4	0.17
(1,142)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	13	0.17
(1,126)	1:23:A:VAL:HA	1:24:A:ASP:H	6	0.17
(1,107)	1:21:A:ARG:HB3	1:25:A:LEU:HD21	8	0.17
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	15	0.17
(1,84)	1:20:A:LEU:HD11	1:23:A:VAL:HG11	3	0.17
(1,84)	1:20:A:LEU:HD12	1:23:A:VAL:HG11	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:20:A:LEU:HD13	1:23:A:VAL:HG11	3	0.17
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	14	0.17
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	14	0.17
(1,69)	1:19:A:TRP:H	1:20:A:LEU:HG	5	0.17
(1,8)	1:11:A:MET:HA	1:12:A:ALA:H	7	0.17
(1,1068)	1:104:A:LEU:HD11	1:106:A:LYS:H	11	0.16
(1,1068)	1:104:A:LEU:HD12	1:106:A:LYS:H	11	0.16
(1,1068)	1:104:A:LEU:HD13	1:106:A:LYS:H	11	0.16
(1,1055)	1:104:A:LEU:HA	1:105:A:LEU:H	13	0.16
(1,1044)	1:103:A:VAL:HG21	1:104:A:LEU:HD21	10	0.16
(1,1028)	1:103:A:VAL:HA	1:104:A:LEU:H	15	0.16
(1,1020)	1:102:A:GLU:HA	1:105:A:LEU:H	9	0.16
(1,1014)	1:102:A:GLU:HA	1:103:A:VAL:H	2	0.16
(1,1006)	1:101:A:GLU:HA	1:104:A:LEU:H	3	0.16
(1,976)	1:100:A:LEU:HA	1:101:A:GLU:H	10	0.16
(1,976)	1:100:A:LEU:HA	1:101:A:GLU:H	13	0.16
(1,933)	1:96:A:LEU:HD22	1:99:A:TRP:HB2	14	0.16
(1,933)	1:96:A:LEU:HD23	1:99:A:TRP:HB2	14	0.16
(1,921)	1:96:A:LEU:H	1:98:A:GLN:H	2	0.16
(1,909)	1:95:A:GLU:HA	1:96:A:LEU:H	4	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG11	1	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG12	1	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG13	1	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG21	1	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG22	1	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG23	1	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG11	9	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG12	9	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG13	9	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG21	9	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG22	9	0.16
(1,884)	1:92:A:ALA:HA	1:94:A:VAL:HG23	9	0.16
(1,786)	1:78:A:GLY:H	1:81:A:THR:H	15	0.16
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	2	0.16
(1,782)	1:78:A:GLY:H	1:80:A:ALA:H	6	0.16
(1,757)	1:72:A:LYS:HA	1:73:A:ASN:H	1	0.16
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	11	0.16
(1,735)	1:70:A:GLU:HA	1:71:A:LEU:H	1	0.16
(1,695)	1:65:A:GLU:HA	1:66:A:MET:H	14	0.16
(1,677)	1:62:A:LEU:HD22	1:64:A:GLY:H	11	0.16
(1,677)	1:62:A:LEU:HD23	1:64:A:GLY:H	11	0.16
(1,636)	1:60:A:GLU:HA	1:61:A:LEU:H	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	1	0.16
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	1	0.16
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	1	0.16
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	1	0.16
(1,607)	1:58:A:VAL:HG23	1:96:A:LEU:HD22	15	0.16
(1,607)	1:58:A:VAL:HG23	1:96:A:LEU:HD23	15	0.16
(1,553)	1:57:A:ILE:HA	1:58:A:VAL:H	13	0.16
(1,551)	1:56:A:ARG:HG3	1:60:A:GLU:H	7	0.16
(1,551)	1:56:A:ARG:HG2	1:60:A:GLU:H	7	0.16
(1,549)	1:56:A:ARG:HA	1:59:A:GLU:H	7	0.16
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	5	0.16
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	5	0.16
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	5	0.16
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	5	0.16
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	5	0.16
(1,492)	1:51:A:LEU:HD11	1:54:A:ARG:HD3	11	0.16
(1,492)	1:51:A:LEU:HD12	1:54:A:ARG:HD3	11	0.16
(1,492)	1:51:A:LEU:HD13	1:54:A:ARG:HD3	11	0.16
(1,486)	1:51:A:LEU:HD11	1:54:A:ARG:H	13	0.16
(1,486)	1:51:A:LEU:HD12	1:54:A:ARG:H	13	0.16
(1,486)	1:51:A:LEU:HD13	1:54:A:ARG:H	13	0.16
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	15	0.16
(1,459)	1:50:A:ALA:HA	1:51:A:LEU:H	4	0.16
(1,454)	1:49:A:GLU:HA	1:50:A:ALA:H	5	0.16
(1,437)	1:47:A:GLU:H	1:48:A:ARG:HB3	14	0.16
(1,437)	1:47:A:GLU:H	1:48:A:ARG:HB2	14	0.16
(1,380)	1:39:A:LEU:HA	1:40:A:ASN:H	14	0.16
(1,369)	1:38:A:LEU:HD22	1:41:A:LEU:H	3	0.16
(1,369)	1:38:A:LEU:HD23	1:41:A:LEU:H	3	0.16
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD22	3	0.16
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD23	3	0.16
(1,336)	1:36:A:LEU:H	1:37:A:PRO:HG3	3	0.16
(1,336)	1:36:A:LEU:H	1:37:A:PRO:HG2	3	0.16
(1,294)	1:35:A:HIS:HA	1:36:A:LEU:H	9	0.16
(1,214)	1:27:A:LYS:HA	1:30:A:TYR:HE1	15	0.16
(1,197)	1:26:A:LEU:HD21	1:29:A:ALA:HB2	9	0.16
(1,191)	1:26:A:LEU:HA	1:29:A:ALA:H	9	0.16
(1,167)	1:25:A:LEU:HA	1:26:A:LEU:H	11	0.16
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD22	6	0.16
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD23	6	0.16
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD11	5	0.16
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD12	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD13	5	0.16
(1,157)	1:24:A:ASP:HA	1:25:A:LEU:H	4	0.16
(1,144)	1:23:A:VAL:HG13	1:26:A:LEU:HD21	10	0.16
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD11	5	0.16
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD12	5	0.16
(1,136)	1:23:A:VAL:HB	1:26:A:LEU:HD13	5	0.16
(1,124)	1:22:A:PHE:HA	1:26:A:LEU:H	14	0.16
(1,109)	1:21:A:ARG:HB2	1:25:A:LEU:HD21	1	0.16
(1,103)	1:21:A:ARG:HA	1:24:A:ASP:H	11	0.16
(1,100)	1:21:A:ARG:HA	1:22:A:PHE:HA	8	0.16
(1,99)	1:21:A:ARG:HA	1:22:A:PHE:H	5	0.16
(1,84)	1:20:A:LEU:HD11	1:23:A:VAL:HG11	4	0.16
(1,84)	1:20:A:LEU:HD12	1:23:A:VAL:HG11	4	0.16
(1,84)	1:20:A:LEU:HD13	1:23:A:VAL:HG11	4	0.16
(1,84)	1:20:A:LEU:HD11	1:23:A:VAL:HG11	9	0.16
(1,84)	1:20:A:LEU:HD12	1:23:A:VAL:HG11	9	0.16
(1,84)	1:20:A:LEU:HD13	1:23:A:VAL:HG11	9	0.16
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	4	0.16
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	4	0.16
(1,49)	1:18:A:GLU:HA	1:21:A:ARG:H	13	0.16
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	2	0.16
(1,40)	1:18:A:GLU:HA	1:19:A:TRP:H	11	0.16
(1,1074)	1:105:A:LEU:HG	1:106:A:LYS:H	2	0.15
(1,1061)	1:104:A:LEU:HB3	1:105:A:LEU:HD21	1	0.15
(1,1061)	1:104:A:LEU:HB2	1:105:A:LEU:HD21	1	0.15
(1,1008)	1:101:A:GLU:HA	1:105:A:LEU:H	10	0.15
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	13	0.15
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	13	0.15
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	13	0.15
(1,972)	1:99:A:TRP:HA	1:102:A:GLU:H	3	0.15
(1,968)	1:99:A:TRP:HA	1:100:A:LEU:H	2	0.15
(1,897)	1:94:A:VAL:HA	1:95:A:GLU:H	9	0.15
(1,892)	1:93:A:PRO:HG3	1:94:A:VAL:H	2	0.15
(1,892)	1:93:A:PRO:HG2	1:94:A:VAL:H	2	0.15
(1,867)	1:90:A:LYS:HA	1:91:A:ALA:H	15	0.15
(1,824)	1:87:A:ASN:HA	1:88:A:SER:H	1	0.15
(1,824)	1:87:A:ASN:HA	1:88:A:SER:H	9	0.15
(1,786)	1:78:A:GLY:H	1:81:A:THR:H	13	0.15
(1,735)	1:70:A:GLU:HA	1:71:A:LEU:H	11	0.15
(1,695)	1:65:A:GLU:HA	1:66:A:MET:H	3	0.15
(1,693)	1:64:A:GLY:HA3	1:66:A:MET:HA	5	0.15
(1,693)	1:64:A:GLY:HA2	1:66:A:MET:HA	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:63:A:ARG:HA	1:64:A:GLY:H	9	0.15
(1,632)	1:59:A:GLU:HG2	1:104:A:LEU:HD21	4	0.15
(1,553)	1:57:A:ILE:HA	1:58:A:VAL:H	5	0.15
(1,490)	1:51:A:LEU:HD21	1:54:A:ARG:HA	7	0.15
(1,486)	1:51:A:LEU:HD11	1:54:A:ARG:H	1	0.15
(1,486)	1:51:A:LEU:HD12	1:54:A:ARG:H	1	0.15
(1,486)	1:51:A:LEU:HD13	1:54:A:ARG:H	1	0.15
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	1	0.15
(1,475)	1:51:A:LEU:HA	1:52:A:GLY:H	8	0.15
(1,447)	1:48:A:ARG:HA	1:49:A:GLU:H	13	0.15
(1,439)	1:47:A:GLU:HA	1:48:A:ARG:H	5	0.15
(1,421)	1:43:A:LEU:HD22	1:48:A:ARG:HD2	11	0.15
(1,421)	1:43:A:LEU:HD23	1:48:A:ARG:HD2	11	0.15
(1,398)	1:41:A:LEU:HA	1:42:A:MET:H	5	0.15
(1,361)	1:38:A:LEU:HA	1:39:A:LEU:H	11	0.15
(1,361)	1:38:A:LEU:HA	1:39:A:LEU:H	15	0.15
(1,294)	1:35:A:HIS:HA	1:36:A:LEU:H	5	0.15
(1,278)	1:33:A:ASP:H	1:34:A:LEU:HG	7	0.15
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD22	14	0.15
(1,267)	1:32:A:ASN:HA	1:34:A:LEU:HD23	14	0.15
(1,243)	1:30:A:TYR:HA	1:31:A:GLN:H	14	0.15
(1,219)	1:28:A:ASN:HA	1:29:A:ALA:H	13	0.15
(1,181)	1:25:A:LEU:HD22	1:28:A:ASN:HB2	7	0.15
(1,181)	1:25:A:LEU:HD23	1:28:A:ASN:HB2	7	0.15
(1,172)	1:25:A:LEU:HA	1:28:A:ASN:H	8	0.15
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD22	11	0.15
(1,165)	1:24:A:ASP:H	1:25:A:LEU:HD23	11	0.15
(1,142)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	9	0.15
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	2	0.15
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	2	0.15
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	2	0.15
(1,44)	1:18:A:GLU:HA	1:19:A:TRP:HA	11	0.15
(1,10)	1:12:A:ALA:HA	1:13:A:GLU:H	6	0.15
(1,1076)	1:105:A:LEU:HD21	1:106:A:LYS:H	2	0.14
(1,1046)	1:103:A:VAL:HG22	1:104:A:LEU:HD21	13	0.14
(1,981)	1:100:A:LEU:HD11	1:102:A:GLU:H	7	0.14
(1,981)	1:100:A:LEU:HD12	1:102:A:GLU:H	7	0.14
(1,981)	1:100:A:LEU:HD13	1:102:A:GLU:H	7	0.14
(1,974)	1:99:A:TRP:HA	1:103:A:VAL:H	10	0.14
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB3	8	0.14
(1,971)	1:99:A:TRP:HA	1:101:A:GLU:HB2	8	0.14
(1,968)	1:99:A:TRP:HA	1:100:A:LEU:H	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,968)	1:99:A:TRP:HA	1:100:A:LEU:H	7	0.14
(1,860)	1:89:A:LEU:HD21	1:92:A:ALA:HB1	8	0.14
(1,835)	1:88:A:SER:HA	1:89:A:LEU:HA	5	0.14
(1,831)	1:88:A:SER:HA	1:89:A:LEU:H	8	0.14
(1,738)	1:70:A:GLU:HG3	1:71:A:LEU:HB3	1	0.14
(1,738)	1:70:A:GLU:HG3	1:71:A:LEU:HB2	1	0.14
(1,738)	1:70:A:GLU:HG2	1:71:A:LEU:HB3	1	0.14
(1,738)	1:70:A:GLU:HG2	1:71:A:LEU:HB2	1	0.14
(1,735)	1:70:A:GLU:HA	1:71:A:LEU:H	2	0.14
(1,717)	1:67:A:SER:HA	1:70:A:GLU:H	6	0.14
(1,649)	1:61:A:LEU:HA	1:62:A:LEU:H	5	0.14
(1,575)	1:58:A:VAL:HA	1:61:A:LEU:HD21	15	0.14
(1,553)	1:57:A:ILE:HA	1:58:A:VAL:H	7	0.14
(1,475)	1:51:A:LEU:HA	1:52:A:GLY:H	14	0.14
(1,443)	1:47:A:GLU:HA	1:50:A:ALA:H	5	0.14
(1,435)	1:46:A:ASP:HA	1:49:A:GLU:H	8	0.14
(1,431)	1:46:A:ASP:HA	1:47:A:GLU:H	5	0.14
(1,366)	1:38:A:LEU:HA	1:41:A:LEU:H	4	0.14
(1,361)	1:38:A:LEU:HA	1:39:A:LEU:H	10	0.14
(1,361)	1:38:A:LEU:HA	1:39:A:LEU:H	12	0.14
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD11	2	0.14
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD12	2	0.14
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD13	2	0.14
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD11	6	0.14
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD12	6	0.14
(1,345)	1:37:A:PRO:HA	1:38:A:LEU:HD13	6	0.14
(1,297)	1:35:A:HIS:HE1	1:36:A:LEU:H	5	0.14
(1,279)	1:33:A:ASP:H	1:35:A:HIS:H	15	0.14
(1,272)	1:32:A:ASN:HB2	1:34:A:LEU:HD21	4	0.14
(1,243)	1:30:A:TYR:HA	1:31:A:GLN:H	4	0.14
(1,229)	1:29:A:ALA:HA	1:32:A:ASN:H	8	0.14
(1,226)	1:29:A:ALA:HA	1:30:A:TYR:H	8	0.14
(1,219)	1:28:A:ASN:HA	1:29:A:ALA:H	3	0.14
(1,219)	1:28:A:ASN:HA	1:29:A:ALA:H	11	0.14
(1,206)	1:27:A:LYS:HA	1:28:A:ASN:H	15	0.14
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG3	10	0.14
(1,187)	1:26:A:LEU:HG	1:27:A:LYS:HG2	10	0.14
(1,181)	1:25:A:LEU:HD22	1:28:A:ASN:HB2	6	0.14
(1,181)	1:25:A:LEU:HD23	1:28:A:ASN:HB2	6	0.14
(1,174)	1:25:A:LEU:HD11	1:28:A:ASN:HA	9	0.14
(1,174)	1:25:A:LEU:HD12	1:28:A:ASN:HA	9	0.14
(1,174)	1:25:A:LEU:HD13	1:28:A:ASN:HA	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	1:25:A:LEU:HA	1:26:A:LEU:H	8	0.14
(1,157)	1:24:A:ASP:HA	1:25:A:LEU:H	2	0.14
(1,126)	1:23:A:VAL:HA	1:24:A:ASP:H	10	0.14
(1,97)	1:20:A:LEU:HA	1:24:A:ASP:H	5	0.14
(1,71)	1:19:A:TRP:H	1:20:A:LEU:HD21	4	0.14
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	10	0.14
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	10	0.14
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	10	0.14
(1,40)	1:18:A:GLU:HA	1:19:A:TRP:H	1	0.14
(1,21)	1:16:A:HIS:HA	1:18:A:GLU:H	7	0.14
(1,10)	1:12:A:ALA:HA	1:13:A:GLU:H	7	0.14
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB3	12	0.13
(1,1078)	1:105:A:LEU:HA	1:106:A:LYS:HB2	12	0.13
(1,1070)	1:104:A:LEU:HD22	1:106:A:LYS:H	14	0.13
(1,1070)	1:104:A:LEU:HD23	1:106:A:LYS:H	14	0.13
(1,1028)	1:103:A:VAL:HA	1:104:A:LEU:H	7	0.13
(1,972)	1:99:A:TRP:HA	1:102:A:GLU:H	13	0.13
(1,928)	1:96:A:LEU:HD22	1:99:A:TRP:H	7	0.13
(1,928)	1:96:A:LEU:HD23	1:99:A:TRP:H	7	0.13
(1,924)	1:96:A:LEU:HD22	1:98:A:GLN:H	11	0.13
(1,924)	1:96:A:LEU:HD23	1:98:A:GLN:H	11	0.13
(1,892)	1:93:A:PRO:HG3	1:94:A:VAL:H	7	0.13
(1,892)	1:93:A:PRO:HG2	1:94:A:VAL:H	7	0.13
(1,867)	1:90:A:LYS:HA	1:91:A:ALA:H	12	0.13
(1,858)	1:89:A:LEU:HD22	1:92:A:ALA:H	11	0.13
(1,858)	1:89:A:LEU:HD23	1:92:A:ALA:H	11	0.13
(1,831)	1:88:A:SER:HA	1:89:A:LEU:H	9	0.13
(1,824)	1:87:A:ASN:HA	1:88:A:SER:H	5	0.13
(1,802)	1:80:A:ALA:H	1:82:A:ILE:HB	7	0.13
(1,763)	1:73:A:ASN:HA	1:74:A:GLU:HB3	8	0.13
(1,763)	1:73:A:ASN:HA	1:74:A:GLU:HB2	8	0.13
(1,762)	1:73:A:ASN:HA	1:74:A:GLU:H	9	0.13
(1,742)	1:70:A:GLU:HG2	1:71:A:LEU:HD21	10	0.13
(1,738)	1:70:A:GLU:HG3	1:71:A:LEU:HB3	3	0.13
(1,738)	1:70:A:GLU:HG3	1:71:A:LEU:HB2	3	0.13
(1,738)	1:70:A:GLU:HG2	1:71:A:LEU:HB3	3	0.13
(1,738)	1:70:A:GLU:HG2	1:71:A:LEU:HB2	3	0.13
(1,703)	1:66:A:MET:HA	1:67:A:SER:HA	2	0.13
(1,675)	1:62:A:LEU:HD11	1:64:A:GLY:H	9	0.13
(1,675)	1:62:A:LEU:HD12	1:64:A:GLY:H	9	0.13
(1,675)	1:62:A:LEU:HD13	1:64:A:GLY:H	9	0.13
(1,674)	1:62:A:LEU:HG	1:63:A:ARG:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,649)	1:61:A:LEU:HA	1:62:A:LEU:H	2	0.13
(1,649)	1:61:A:LEU:HA	1:62:A:LEU:H	9	0.13
(1,632)	1:59:A:GLU:HG2	1:104:A:LEU:HD21	11	0.13
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	14	0.13
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	14	0.13
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	14	0.13
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	14	0.13
(1,596)	1:58:A:VAL:HG11	1:96:A:LEU:HD21	10	0.13
(1,535)	1:55:A:VAL:HA	1:56:A:ARG:H	9	0.13
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	12	0.13
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	12	0.13
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	12	0.13
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	12	0.13
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	12	0.13
(1,475)	1:51:A:LEU:HA	1:52:A:GLY:H	13	0.13
(1,447)	1:48:A:ARG:HA	1:49:A:GLU:H	9	0.13
(1,439)	1:47:A:GLU:HA	1:48:A:ARG:H	13	0.13
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	10	0.13
(1,421)	1:43:A:LEU:HD22	1:48:A:ARG:HD2	5	0.13
(1,421)	1:43:A:LEU:HD23	1:48:A:ARG:HD2	5	0.13
(1,405)	1:42:A:MET:H	1:43:A:LEU:HG	7	0.13
(1,373)	1:38:A:LEU:HA	1:42:A:MET:H	9	0.13
(1,361)	1:38:A:LEU:HA	1:39:A:LEU:H	3	0.13
(1,361)	1:38:A:LEU:HA	1:39:A:LEU:H	9	0.13
(1,328)	1:36:A:LEU:HD21	1:39:A:LEU:HD21	14	0.13
(1,294)	1:35:A:HIS:HA	1:36:A:LEU:H	3	0.13
(1,223)	1:28:A:ASN:HA	1:32:A:ASN:H	11	0.13
(1,213)	1:27:A:LYS:HA	1:30:A:TYR:HD1	1	0.13
(1,206)	1:27:A:LYS:HA	1:28:A:ASN:H	12	0.13
(1,205)	1:27:A:LYS:H	1:28:A:ASN:H	8	0.13
(1,191)	1:26:A:LEU:HA	1:29:A:ALA:H	3	0.13
(1,191)	1:26:A:LEU:HA	1:29:A:ALA:H	14	0.13
(1,167)	1:25:A:LEU:HA	1:26:A:LEU:H	3	0.13
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD11	10	0.13
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD12	10	0.13
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD13	10	0.13
(1,158)	1:24:A:ASP:HA	1:27:A:LYS:H	5	0.13
(1,98)	1:21:A:ARG:H	1:22:A:PHE:H	13	0.13
(1,81)	1:20:A:LEU:HB3	1:22:A:PHE:H	3	0.13
(1,81)	1:20:A:LEU:HB2	1:22:A:PHE:H	3	0.13
(1,78)	1:20:A:LEU:HA	1:21:A:ARG:H	12	0.13
(1,71)	1:19:A:TRP:H	1:20:A:LEU:HD21	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:18:A:GLU:HA	1:19:A:TRP:H	12	0.13
(1,30)	1:17:A:GLN:HA	1:18:A:GLU:HA	6	0.13
(1,21)	1:16:A:HIS:HA	1:18:A:GLU:H	1	0.13
(1,8)	1:11:A:MET:HA	1:12:A:ALA:H	9	0.13
(1,1051)	1:103:A:VAL:HA	1:105:A:LEU:H	8	0.12
(1,1028)	1:103:A:VAL:HA	1:104:A:LEU:H	13	0.12
(1,984)	1:100:A:LEU:HA	1:103:A:VAL:H	8	0.12
(1,976)	1:100:A:LEU:HA	1:101:A:GLU:H	14	0.12
(1,968)	1:99:A:TRP:HA	1:100:A:LEU:H	11	0.12
(1,962)	1:98:A:GLN:HA	1:99:A:TRP:H	6	0.12
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD22	2	0.12
(1,958)	1:97:A:ARG:HA	1:100:A:LEU:HD23	2	0.12
(1,856)	1:89:A:LEU:HD11	1:92:A:ALA:H	2	0.12
(1,856)	1:89:A:LEU:HD12	1:92:A:ALA:H	2	0.12
(1,856)	1:89:A:LEU:HD13	1:92:A:ALA:H	2	0.12
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD11	14	0.12
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD12	14	0.12
(1,768)	1:75:A:LEU:HB3	1:79:A:ILE:HD13	14	0.12
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD11	14	0.12
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD12	14	0.12
(1,768)	1:75:A:LEU:HB2	1:79:A:ILE:HD13	14	0.12
(1,762)	1:73:A:ASN:HA	1:74:A:GLU:H	10	0.12
(1,735)	1:70:A:GLU:HA	1:71:A:LEU:H	7	0.12
(1,695)	1:65:A:GLU:HA	1:66:A:MET:H	6	0.12
(1,691)	1:64:A:GLY:H	1:66:A:MET:H	8	0.12
(1,650)	1:61:A:LEU:HA	1:64:A:GLY:H	9	0.12
(1,649)	1:61:A:LEU:HA	1:62:A:LEU:H	4	0.12
(1,644)	1:60:A:GLU:H	1:61:A:LEU:HD22	3	0.12
(1,644)	1:60:A:GLU:H	1:61:A:LEU:HD23	3	0.12
(1,623)	1:59:A:GLU:HA	1:104:A:LEU:HD22	2	0.12
(1,623)	1:59:A:GLU:HA	1:104:A:LEU:HD23	2	0.12
(1,600)	1:58:A:VAL:HG13	1:96:A:LEU:HD21	11	0.12
(1,596)	1:58:A:VAL:HG11	1:96:A:LEU:HD21	15	0.12
(1,588)	1:58:A:VAL:HG21	1:61:A:LEU:HD21	2	0.12
(1,550)	1:56:A:ARG:HA	1:60:A:GLU:H	1	0.12
(1,535)	1:55:A:VAL:HA	1:56:A:ARG:H	8	0.12
(1,486)	1:51:A:LEU:HD11	1:54:A:ARG:H	8	0.12
(1,486)	1:51:A:LEU:HD12	1:54:A:ARG:H	8	0.12
(1,486)	1:51:A:LEU:HD13	1:54:A:ARG:H	8	0.12
(1,459)	1:50:A:ALA:HA	1:51:A:LEU:H	10	0.12
(1,454)	1:49:A:GLU:HA	1:50:A:ALA:H	13	0.12
(1,439)	1:47:A:GLU:HA	1:48:A:ARG:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,428)	1:45:A:PRO:HB3	1:47:A:GLU:H	13	0.12
(1,428)	1:45:A:PRO:HB2	1:47:A:GLU:H	13	0.12
(1,400)	1:41:A:LEU:HD21	1:42:A:MET:H	5	0.12
(1,380)	1:39:A:LEU:HA	1:40:A:ASN:H	2	0.12
(1,361)	1:38:A:LEU:HA	1:39:A:LEU:H	6	0.12
(1,336)	1:36:A:LEU:H	1:37:A:PRO:HG3	7	0.12
(1,336)	1:36:A:LEU:H	1:37:A:PRO:HG2	7	0.12
(1,294)	1:35:A:HIS:HA	1:36:A:LEU:H	2	0.12
(1,294)	1:35:A:HIS:HA	1:36:A:LEU:H	10	0.12
(1,294)	1:35:A:HIS:HA	1:36:A:LEU:H	13	0.12
(1,243)	1:30:A:TYR:HA	1:31:A:GLN:H	5	0.12
(1,226)	1:29:A:ALA:HA	1:30:A:TYR:H	6	0.12
(1,197)	1:26:A:LEU:HD21	1:29:A:ALA:HB2	7	0.12
(1,189)	1:26:A:LEU:HD21	1:27:A:LYS:H	15	0.12
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD11	11	0.12
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD12	11	0.12
(1,163)	1:24:A:ASP:H	1:25:A:LEU:HD13	11	0.12
(1,158)	1:24:A:ASP:HA	1:27:A:LYS:H	14	0.12
(1,146)	1:23:A:VAL:HG21	1:26:A:LEU:HD21	15	0.12
(1,114)	1:22:A:PHE:HA	1:25:A:LEU:H	12	0.12
(1,80)	1:20:A:LEU:H	1:22:A:PHE:H	9	0.12
(1,78)	1:20:A:LEU:HA	1:21:A:ARG:H	11	0.12
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	13	0.12
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	13	0.12
(1,76)	1:20:A:LEU:HD21	1:21:A:ARG:H	1	0.12
(1,40)	1:18:A:GLU:HA	1:19:A:TRP:H	3	0.12
(1,8)	1:11:A:MET:HA	1:12:A:ALA:H	15	0.12
(1,1055)	1:104:A:LEU:HA	1:105:A:LEU:H	10	0.11
(1,1028)	1:103:A:VAL:HA	1:104:A:LEU:H	5	0.11
(1,1014)	1:102:A:GLU:HA	1:103:A:VAL:H	7	0.11
(1,1014)	1:102:A:GLU:HA	1:103:A:VAL:H	15	0.11
(1,982)	1:100:A:LEU:HD21	1:102:A:GLU:H	10	0.11
(1,976)	1:100:A:LEU:HA	1:101:A:GLU:H	6	0.11
(1,968)	1:99:A:TRP:HA	1:100:A:LEU:H	13	0.11
(1,968)	1:99:A:TRP:HA	1:100:A:LEU:H	14	0.11
(1,962)	1:98:A:GLN:HA	1:99:A:TRP:H	1	0.11
(1,951)	1:97:A:ARG:HA	1:98:A:GLN:H	15	0.11
(1,924)	1:96:A:LEU:HD22	1:98:A:GLN:H	2	0.11
(1,924)	1:96:A:LEU:HD23	1:98:A:GLN:H	2	0.11
(1,924)	1:96:A:LEU:HD22	1:98:A:GLN:H	3	0.11
(1,924)	1:96:A:LEU:HD23	1:98:A:GLN:H	3	0.11
(1,875)	1:91:A:ALA:HA	1:92:A:ALA:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,867)	1:90:A:LYS:HA	1:91:A:ALA:H	4	0.11
(1,762)	1:73:A:ASN:HA	1:74:A:GLU:H	13	0.11
(1,735)	1:70:A:GLU:HA	1:71:A:LEU:H	10	0.11
(1,674)	1:62:A:LEU:HG	1:63:A:ARG:H	2	0.11
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG3	5	0.11
(1,617)	1:59:A:GLU:HG3	1:65:A:GLU:HG2	5	0.11
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG3	5	0.11
(1,617)	1:59:A:GLU:HG2	1:65:A:GLU:HG2	5	0.11
(1,604)	1:58:A:VAL:HG22	1:96:A:LEU:HD21	11	0.11
(1,553)	1:57:A:ILE:HA	1:58:A:VAL:H	15	0.11
(1,535)	1:55:A:VAL:HA	1:56:A:ARG:H	4	0.11
(1,500)	1:51:A:LEU:HD22	1:55:A:VAL:HG11	11	0.11
(1,500)	1:51:A:LEU:HD23	1:55:A:VAL:HG11	11	0.11
(1,500)	1:51:A:LEU:HD11	1:55:A:VAL:HG12	11	0.11
(1,500)	1:51:A:LEU:HD12	1:55:A:VAL:HG12	11	0.11
(1,500)	1:51:A:LEU:HD13	1:55:A:VAL:HG12	11	0.11
(1,478)	1:51:A:LEU:HG	1:52:A:GLY:H	7	0.11
(1,459)	1:50:A:ALA:HA	1:51:A:LEU:H	9	0.11
(1,454)	1:49:A:GLU:HA	1:50:A:ALA:H	4	0.11
(1,454)	1:49:A:GLU:HA	1:50:A:ALA:H	12	0.11
(1,437)	1:47:A:GLU:H	1:48:A:ARG:HB3	11	0.11
(1,437)	1:47:A:GLU:H	1:48:A:ARG:HB2	11	0.11
(1,436)	1:46:A:ASP:HA	1:50:A:ALA:H	9	0.11
(1,406)	1:42:A:MET:HA	1:43:A:LEU:H	15	0.11
(1,398)	1:41:A:LEU:HA	1:42:A:MET:H	11	0.11
(1,380)	1:39:A:LEU:HA	1:40:A:ASN:H	1	0.11
(1,380)	1:39:A:LEU:HA	1:40:A:ASN:H	15	0.11
(1,371)	1:38:A:LEU:HA	1:41:A:LEU:HD21	10	0.11
(1,366)	1:38:A:LEU:HA	1:41:A:LEU:H	11	0.11
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD22	8	0.11
(1,352)	1:37:A:PRO:HG2	1:38:A:LEU:HD23	8	0.11
(1,328)	1:36:A:LEU:HD21	1:39:A:LEU:HD21	11	0.11
(1,294)	1:35:A:HIS:HA	1:36:A:LEU:H	8	0.11
(1,243)	1:30:A:TYR:HA	1:31:A:GLN:H	8	0.11
(1,226)	1:29:A:ALA:HA	1:30:A:TYR:H	10	0.11
(1,226)	1:29:A:ALA:HA	1:30:A:TYR:H	13	0.11
(1,219)	1:28:A:ASN:HA	1:29:A:ALA:H	15	0.11
(1,215)	1:27:A:LYS:HA	1:30:A:TYR:H	14	0.11
(1,201)	1:26:A:LEU:HG	1:30:A:TYR:H	12	0.11
(1,142)	1:23:A:VAL:HG12	1:26:A:LEU:HD21	15	0.11
(1,98)	1:21:A:ARG:H	1:22:A:PHE:H	14	0.11
(1,77)	1:20:A:LEU:HD22	1:21:A:ARG:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:20:A:LEU:HD23	1:21:A:ARG:H	8	0.11
(1,66)	1:19:A:TRP:HA	1:23:A:VAL:H	2	0.11
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD11	14	0.11
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD12	14	0.11
(1,60)	1:19:A:TRP:HZ2	1:20:A:LEU:HD13	14	0.11
(1,47)	1:18:A:GLU:HA	1:20:A:LEU:H	13	0.11
(1,40)	1:18:A:GLU:HA	1:19:A:TRP:H	2	0.11
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD22	15	0.11
(1,36)	1:17:A:GLN:HA	1:20:A:LEU:HD23	15	0.11
(1,22)	1:16:A:HIS:HA	1:19:A:TRP:H	11	0.11
(1,1066)	1:104:A:LEU:H	1:106:A:LYS:H	3	0.1
(1,1055)	1:104:A:LEU:HA	1:105:A:LEU:H	2	0.1
(1,1028)	1:103:A:VAL:HA	1:104:A:LEU:H	14	0.1
(1,933)	1:96:A:LEU:HD22	1:99:A:TRP:HB2	15	0.1
(1,933)	1:96:A:LEU:HD23	1:99:A:TRP:HB2	15	0.1
(1,831)	1:88:A:SER:HA	1:89:A:LEU:H	1	0.1
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA3	6	0.1
(1,804)	1:82:A:ILE:H	1:85:A:GLY:HA2	6	0.1
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD22	8	0.1
(1,743)	1:70:A:GLU:HG2	1:71:A:LEU:HD23	8	0.1
(1,717)	1:67:A:SER:HA	1:70:A:GLU:H	1	0.1
(1,693)	1:64:A:GLY:HA3	1:66:A:MET:HA	13	0.1
(1,693)	1:64:A:GLY:HA2	1:66:A:MET:HA	13	0.1
(1,636)	1:60:A:GLU:HA	1:61:A:LEU:H	8	0.1
(1,636)	1:60:A:GLU:HA	1:61:A:LEU:H	14	0.1
(1,588)	1:58:A:VAL:HG21	1:61:A:LEU:HD21	9	0.1
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD22	7	0.1
(1,576)	1:58:A:VAL:HA	1:61:A:LEU:HD23	7	0.1
(1,526)	1:54:A:ARG:HA	1:55:A:VAL:H	7	0.1
(1,398)	1:41:A:LEU:HA	1:42:A:MET:H	14	0.1
(1,353)	1:37:A:PRO:HA	1:40:A:ASN:H	3	0.1
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	14	0.1
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	14	0.1
(1,334)	1:36:A:LEU:HD22	1:39:A:LEU:HD23	15	0.1
(1,334)	1:36:A:LEU:HD23	1:39:A:LEU:HD23	15	0.1
(1,294)	1:35:A:HIS:HA	1:36:A:LEU:H	15	0.1
(1,197)	1:26:A:LEU:HD21	1:29:A:ALA:HB2	13	0.1
(1,181)	1:25:A:LEU:HD22	1:28:A:ASN:HB2	5	0.1
(1,181)	1:25:A:LEU:HD23	1:28:A:ASN:HB2	5	0.1
(1,157)	1:24:A:ASP:HA	1:25:A:LEU:H	7	0.1
(1,126)	1:23:A:VAL:HA	1:24:A:ASP:H	7	0.1
(1,126)	1:23:A:VAL:HA	1:24:A:ASP:H	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:19:A:TRP:H	1:20:A:LEU:HD21	6	0.1
(1,63)	1:19:A:TRP:HA	1:21:A:ARG:H	6	0.1
(1,10)	1:12:A:ALA:HA	1:13:A:GLU:H	13	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found