



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 09:36 AM UTC

PDB ID : 2N3V / pdb_00002n3v
BMRB ID : 25657
Title : Solution structure of the Rpn1 T1 site with K48-linked diubiquitin in the extended binding mode
Authors : Chen, X.; Walters, K.J.
Deposited on : 2015-06-10

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

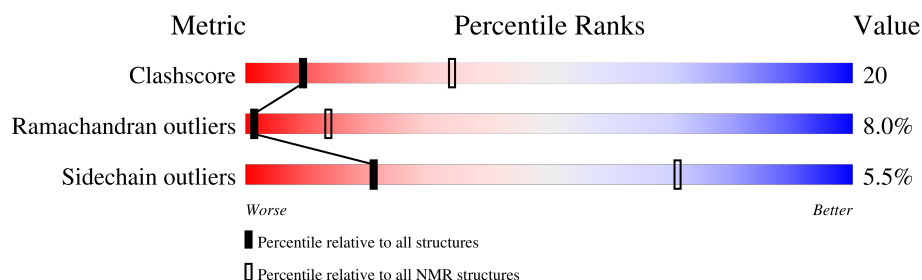
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 27%.

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	131	
2	B	76	
2	C	76	

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:494-A:553, A:561-A:575, A:579-A:607, B:1-B:72, C:1-C:76 (252)	1.06	5

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4380 atoms, of which 2223 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms						Trace
1	A	131	Total	C	H	N	O	S	0
			1921	606	967	150	192	6	

- Molecule 2 is a protein called Ubiquitin-60S ribosomal protein L40.

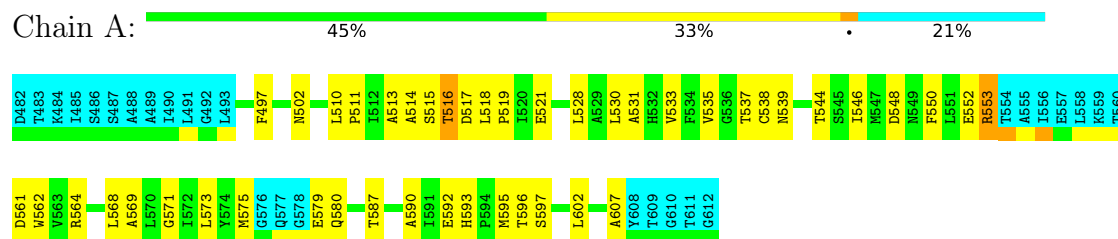
Mol	Chain	Residues	Atoms						Trace
2	B	76	Total	C	H	N	O	S	0
			1229	378	627	105	118	1	
2	C	76	Total	C	H	N	O	S	0
			1230	378	629	105	117	1	

4 Residue-property plots

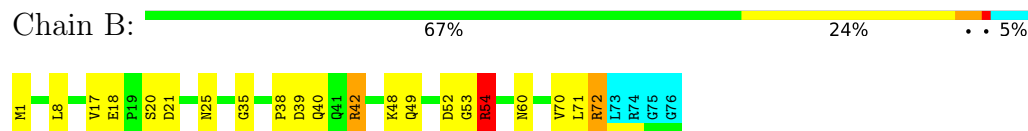
4.1 Average score per residue in the NMR ensemble

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

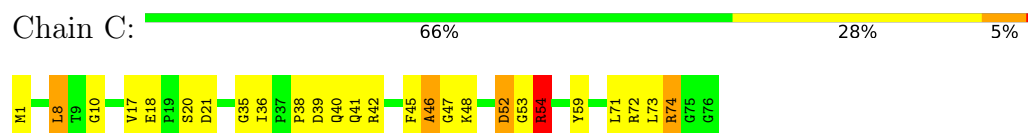
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40



- Molecule 2: Ubiquitin-60S ribosomal protein L40



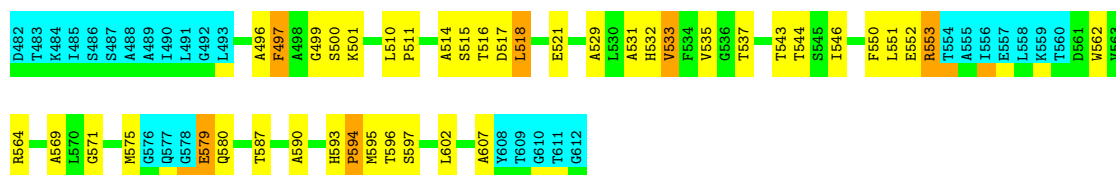
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: 26S proteasome regulatory subunit RPN1





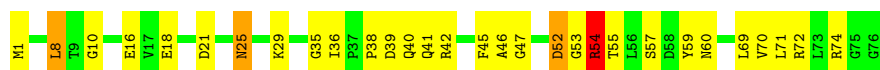
- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain B: 71% 21% 5%



- Molecule 2: Ubiquitin-60S ribosomal protein L40

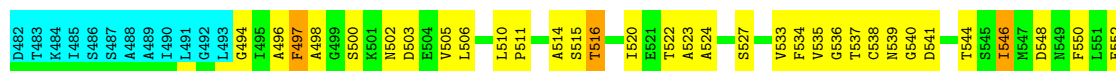
Chain C: 61% 34% 5%



4.2.2 Score per residue for model 2

- Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 42% 31% 7% 21%



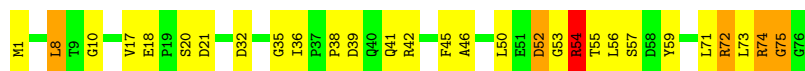
- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain B: 70% 22% 5%



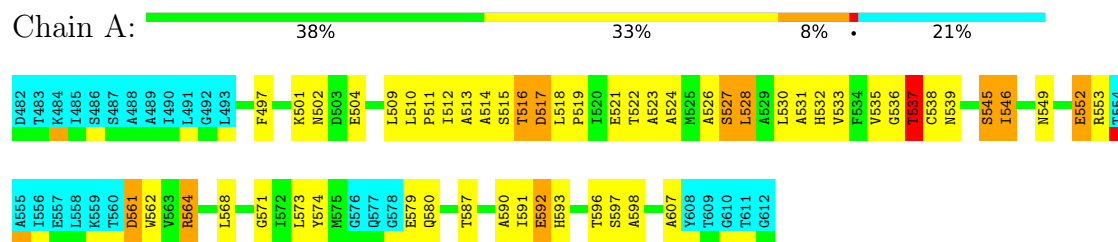
- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain C: 62% 30% 7%

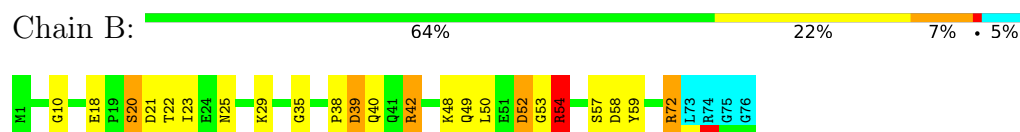


4.2.3 Score per residue for model 3

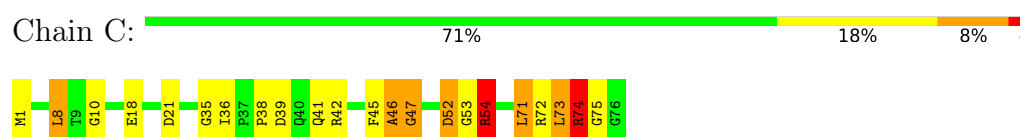
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

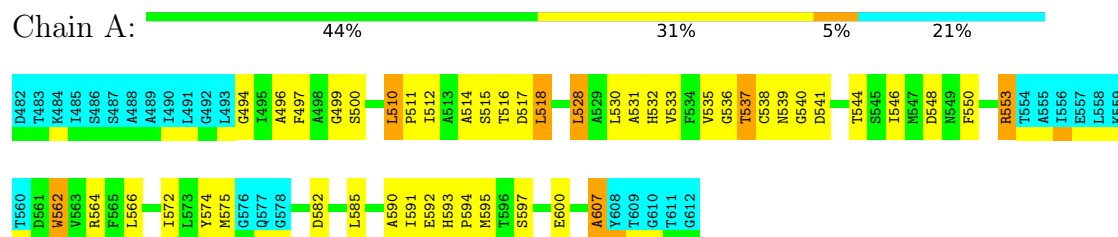


- Molecule 2: Ubiquitin-60S ribosomal protein L40

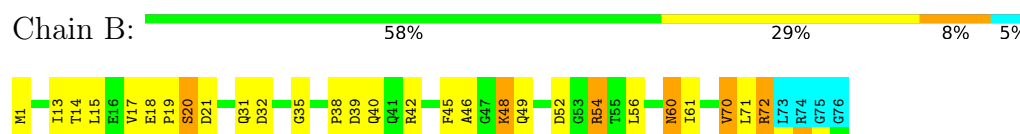


4.2.4 Score per residue for model 4

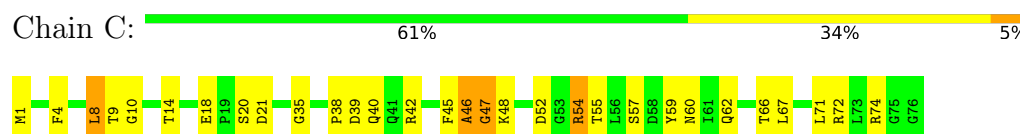
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

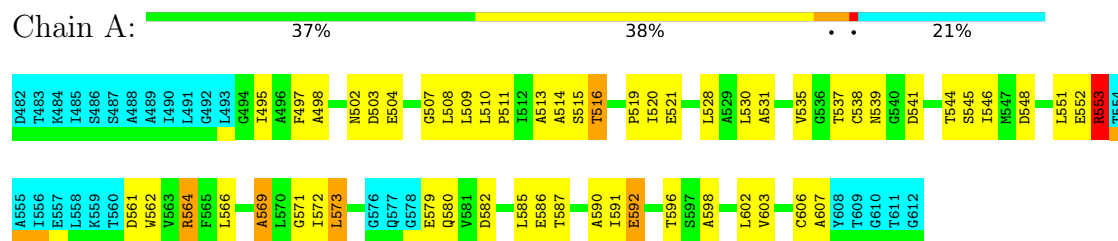


- Molecule 2: Ubiquitin-60S ribosomal protein L40

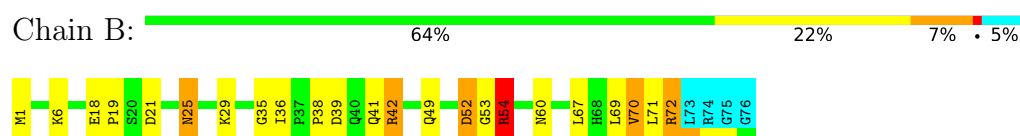


4.2.5 Score per residue for model 5 (medoid)

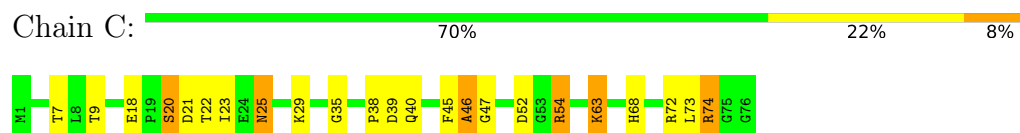
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

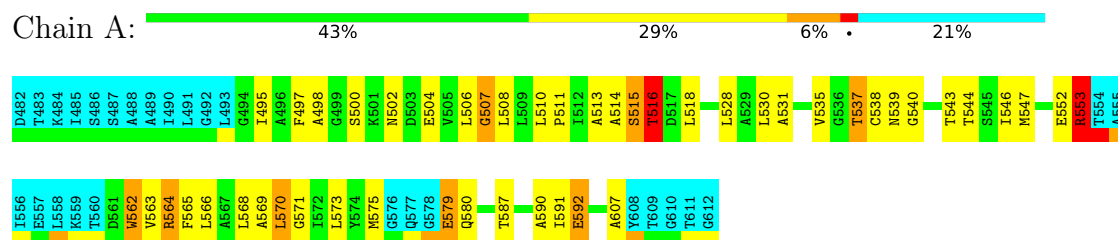


- Molecule 2: Ubiquitin-60S ribosomal protein L40

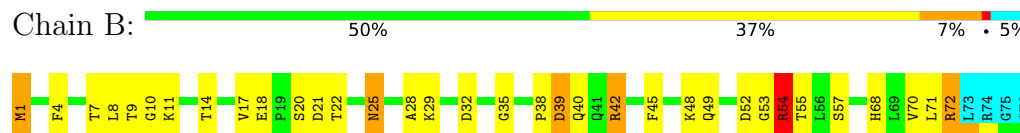


4.2.6 Score per residue for model 6

- Molecule 1: 26S proteasome regulatory subunit RPN1

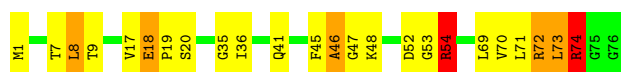


- Molecule 2: Ubiquitin-60S ribosomal protein L40



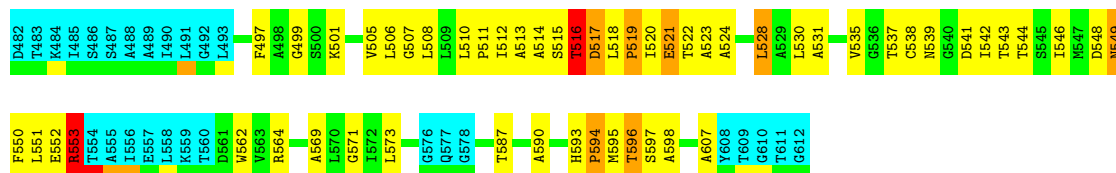
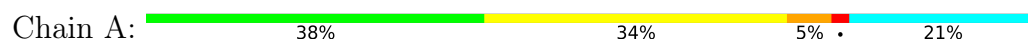
- Molecule 2: Ubiquitin-60S ribosomal protein L40



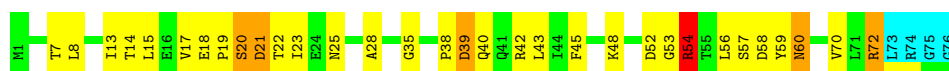


4.2.7 Score per residue for model 7

- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40



- Molecule 2: Ubiquitin-60S ribosomal protein L40

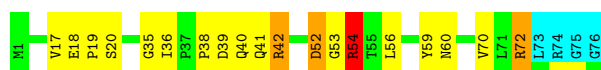


4.2.8 Score per residue for model 8

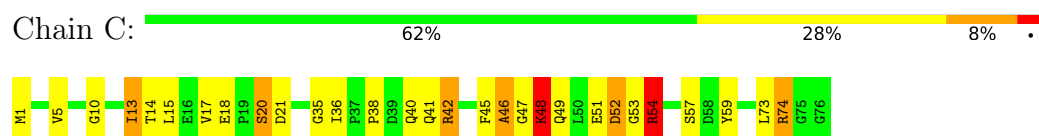
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

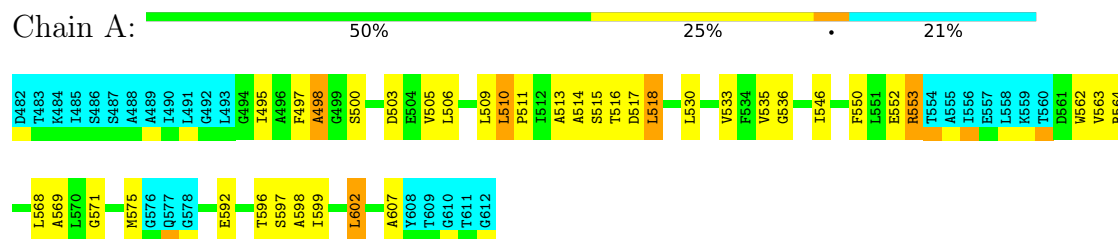


- Molecule 2: Ubiquitin-60S ribosomal protein L40

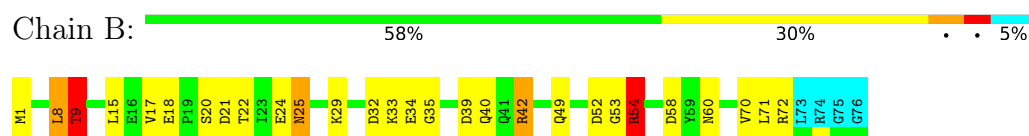


4.2.9 Score per residue for model 9

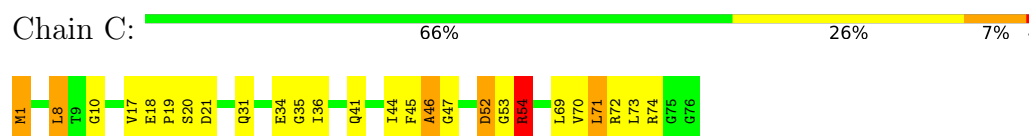
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

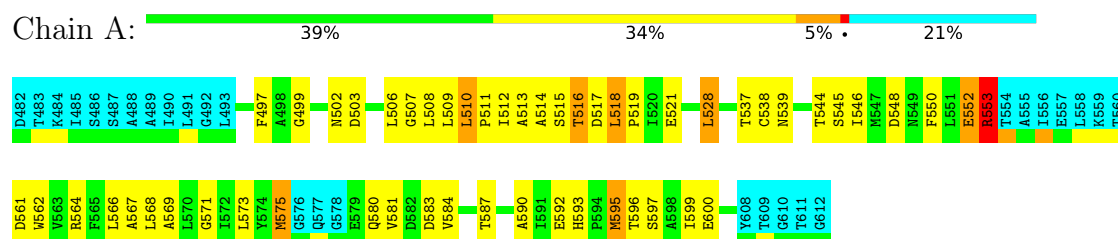


- Molecule 2: Ubiquitin-60S ribosomal protein L40



4.2.10 Score per residue for model 10

- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40





- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain C: 63% 28% 8%



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 10 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
TopSpin	structure solution	
NMRPipe	structure solution	
XEASY	structure solution	
X-PLOR NIH	structure solution	NIH
TALOS	structure solution	
PROCHECKNMR	structure solution	

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	1034
Number of shifts mapped to atoms	1034
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	27%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.53±0.00	0±0/779 (0.0± 0.0%)	0.93±0.01	0±0/1064 (0.0± 0.0%)
2	B	0.55±0.01	0±0/581 (0.0± 0.0%)	1.02±0.01	0±0/784 (0.0± 0.0%)
2	C	0.54±0.00	0±0/607 (0.0± 0.0%)	1.01±0.01	0±0/816 (0.0± 0.0%)
All	All	0.54	0/19670 (0.0%)	0.99	1/26640 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.9±0.3
2	B	0.0±0.0	3.0±0.0
2	C	0.0±0.0	3.3±0.8
All	All	0	82

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	21	ASP	N-CA-C	-6.63	98.83	109.96	7	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	564	ARG	Sidechain	10
2	B	42	ARG	Sidechain	10
2	B	54	ARG	Sidechain	10
2	B	72	ARG	Sidechain	10

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Mol	Chain	Res	Type	Group	Models (Total)
2	C	54	ARG	Sidechain	10
1	A	553	ARG	Sidechain	9
2	C	72	ARG	Sidechain	8
2	C	74	ARG	Sidechain	8
2	C	42	ARG	Sidechain	7

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	767	771	771	42±7
2	B	574	597	597	20±5
2	C	601	629	629	20±3
All	All	19420	19970	19969	793

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 20.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:71:LEU:H	2:C:71:LEU:HD23	0.76	1.41	4	2
2:B:69:LEU:C	2:B:69:LEU:HD23	0.73	2.08	5	1
2:C:69:LEU:C	2:C:69:LEU:HD23	0.73	2.09	9	3
1:A:599:ILE:HD12	1:A:599:ILE:N	0.65	2.06	10	2
2:C:71:LEU:HD12	2:C:71:LEU:N	0.64	2.06	2	1
1:A:510:LEU:O	1:A:514:ALA:N	0.64	2.29	10	5
2:C:71:LEU:HD23	2:C:71:LEU:N	0.64	2.08	1	2
2:B:25:ASN:HD21	2:B:29:LYS:NZ	0.64	1.91	6	3
2:B:25:ASN:ND2	2:B:29:LYS:HZ3	0.63	1.91	6	2
1:A:550:PHE:CE1	1:A:553:ARG:NH2	0.63	2.66	9	1
2:C:71:LEU:H	2:C:71:LEU:CD2	0.62	2.05	4	2
1:A:550:PHE:CZ	1:A:553:ARG:NH2	0.62	2.68	9	1
2:C:54:ARG:N	2:C:54:ARG:NE	0.62	2.48	3	1
2:C:45:PHE:CG	2:C:46:ALA:N	0.62	2.67	10	8
1:A:593:HIS:N	1:A:594:PRO:CD	0.61	2.63	7	1
2:C:25:ASN:ND2	2:C:29:LYS:NZ	0.61	2.47	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:511:PRO:O	1:A:515:SER:N	0.61	2.32	7	3
2:B:38:PRO:C	2:B:40:GLN:H	0.61	2.04	2	4
1:A:518:LEU:N	1:A:518:LEU:CD2	0.61	2.63	1	4
2:C:45:PHE:O	2:C:47:GLY:N	0.60	2.34	6	8
2:B:25:ASN:ND2	2:B:29:LYS:NZ	0.59	2.48	6	4
1:A:552:GLU:O	1:A:553:ARG:O	0.59	2.21	5	4
2:B:49:GLN:NE2	2:B:72:ARG:NH1	0.59	2.50	4	1
1:A:538:CYS:SG	1:A:539:ASN:N	0.58	2.75	2	2
2:C:69:LEU:HD23	2:C:70:VAL:N	0.58	2.12	9	3
2:B:15:LEU:CD2	2:B:33:LYS:NZ	0.58	2.67	9	1
1:A:514:ALA:O	1:A:515:SER:C	0.58	2.47	5	8
2:B:60:ASN:N	2:B:60:ASN:ND2	0.57	2.50	7	1
1:A:515:SER:O	1:A:516:THR:OG1	0.57	2.21	7	6
1:A:510:LEU:CB	1:A:511:PRO:CD	0.57	2.82	10	10
2:B:15:LEU:CD2	2:B:33:LYS:HZ2	0.57	2.12	9	1
2:C:36:ILE:O	2:C:41:GLN:NE2	0.57	2.37	9	6
1:A:553:ARG:NH1	1:A:562:TRP:CH2	0.57	2.73	2	1
2:C:54:ARG:N	2:C:54:ARG:HE	0.56	1.96	3	1
2:B:36:ILE:O	2:B:41:GLN:NE2	0.56	2.38	8	2
1:A:580:GLN:H	1:A:580:GLN:NE2	0.56	1.98	5	1
1:A:502:ASN:N	1:A:502:ASN:OD1	0.56	2.35	8	1
2:C:71:LEU:N	2:C:71:LEU:CD1	0.56	2.68	2	1
1:A:516:THR:OG1	2:B:42:ARG:NH1	0.56	2.39	8	1
1:A:510:LEU:HB3	1:A:511:PRO:CD	0.55	2.31	5	7
1:A:518:LEU:N	1:A:518:LEU:HD22	0.55	2.15	1	3
2:C:71:LEU:HD12	2:C:71:LEU:O	0.55	2.02	9	3
2:B:38:PRO:O	2:B:40:GLN:N	0.55	2.40	10	7
2:B:25:ASN:ND2	2:B:29:LYS:HZ1	0.55	2.00	1	1
2:C:45:PHE:CD2	2:C:46:ALA:N	0.55	2.75	7	4
2:B:40:GLN:CD	2:B:40:GLN:N	0.55	2.65	9	2
2:C:69:LEU:C	2:C:69:LEU:CD2	0.55	2.80	9	3
2:C:18:GLU:H	2:C:21:ASP:CG	0.55	2.09	4	6
2:C:38:PRO:C	2:C:40:GLN:N	0.54	2.65	5	5
2:B:25:ASN:OD1	2:B:29:LYS:NZ	0.54	2.39	3	1
2:B:60:ASN:N	2:B:60:ASN:HD22	0.54	2.00	7	1
2:B:71:LEU:HD22	2:B:71:LEU:N	0.54	2.17	1	1
2:B:71:LEU:N	2:B:71:LEU:CD2	0.54	2.70	1	3
2:B:1:MET:HE1	2:B:61:ILE:O	0.54	2.03	4	1
2:C:45:PHE:O	2:C:46:ALA:C	0.54	2.51	3	6
1:A:562:TRP:CE3	1:A:563:VAL:N	0.54	2.76	6	2
2:B:9:THR:O	2:B:11:LYS:N	0.54	2.41	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:38:PRO:O	2:C:40:GLN:N	0.54	2.40	5	2
2:C:45:PHE:C	2:C:47:GLY:N	0.54	2.65	7	4
1:A:517:ASP:O	1:A:518:LEU:O	0.54	2.26	1	4
2:C:18:GLU:N	2:C:21:ASP:OD2	0.54	2.41	8	2
1:A:552:GLU:N	1:A:552:GLU:CD	0.53	2.66	3	2
1:A:599:ILE:N	1:A:599:ILE:CD1	0.53	2.71	10	2
2:B:38:PRO:C	2:B:40:GLN:N	0.53	2.64	10	7
1:A:592:GLU:O	1:A:593:HIS:ND1	0.53	2.41	2	1
1:A:595:MET:C	1:A:597:SER:N	0.53	2.65	7	4
2:C:16:GLU:N	2:C:16:GLU:CD	0.53	2.67	1	2
1:A:595:MET:O	1:A:597:SER:N	0.53	2.41	7	2
2:B:69:LEU:C	2:B:69:LEU:CD2	0.53	2.79	5	1
2:C:8:LEU:HD23	2:C:8:LEU:O	0.53	2.04	2	7
2:B:18:GLU:O	2:B:20:SER:N	0.53	2.41	4	3
1:A:547:MET:SD	2:C:8:LEU:CD1	0.53	2.97	6	1
1:A:552:GLU:O	1:A:553:ARG:C	0.53	2.52	7	3
1:A:552:GLU:N	1:A:552:GLU:OE1	0.53	2.41	8	2
2:B:18:GLU:H	2:B:21:ASP:CG	0.53	2.11	9	6
2:B:58:ASP:O	2:B:59:TYR:CD1	0.53	2.62	10	3
2:C:45:PHE:O	2:C:48:LYS:N	0.53	2.42	10	1
1:A:522:THR:HG23	1:A:523:ALA:N	0.53	2.19	3	1
1:A:506:LEU:O	1:A:508:LEU:N	0.53	2.41	6	2
2:B:18:GLU:N	2:B:21:ASP:OD2	0.52	2.41	2	1
2:B:70:VAL:C	2:B:71:LEU:HD12	0.52	2.29	4	1
2:C:71:LEU:N	2:C:71:LEU:CD2	0.52	2.72	1	1
1:A:517:ASP:O	2:B:72:ARG:NH2	0.52	2.42	3	1
1:A:538:CYS:O	1:A:539:ASN:ND2	0.52	2.43	6	3
1:A:548:ASP:CG	2:C:72:ARG:O	0.52	2.53	7	2
2:B:42:ARG:NE	2:B:49:GLN:CD	0.52	2.67	6	1
2:C:46:ALA:C	2:C:48:LYS:N	0.52	2.67	4	1
1:A:592:GLU:H	1:A:592:GLU:CD	0.52	2.13	8	1
1:A:537:THR:OG1	1:A:538:CYS:N	0.52	2.41	4	3
1:A:539:ASN:ND2	1:A:541:ASP:OD2	0.52	2.43	5	1
2:C:46:ALA:O	2:C:48:LYS:N	0.52	2.43	4	1
1:A:596:THR:O	1:A:597:SER:C	0.51	2.53	10	3
2:B:42:ARG:HE	2:B:49:GLN:CD	0.51	2.14	6	1
2:B:43:LEU:HD12	2:B:43:LEU:N	0.51	2.20	7	1
1:A:566:LEU:N	1:A:566:LEU:HD12	0.51	2.18	5	3
1:A:539:ASN:ND2	1:A:574:TYR:CE1	0.51	2.78	3	1
2:C:51:GLU:N	2:C:51:GLU:CD	0.51	2.68	8	1
2:B:71:LEU:N	2:B:71:LEU:HD22	0.51	2.21	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:497:PHE:C	1:A:499:GLY:N	0.51	2.67	10	4
2:C:21:ASP:OD1	2:C:21:ASP:N	0.51	2.44	10	1
2:B:48:LYS:NZ	2:C:75:GLY:C	0.51	2.69	2	2
1:A:515:SER:OG	1:A:516:THR:N	0.51	2.43	5	1
1:A:497:PHE:C	1:A:499:GLY:H	0.51	2.14	7	4
2:C:4:PHE:CE2	2:C:14:THR:OG1	0.51	2.60	4	1
1:A:562:TRP:CD2	1:A:563:VAL:N	0.50	2.79	6	2
2:C:38:PRO:C	2:C:40:GLN:H	0.50	2.14	1	5
2:C:71:LEU:CD2	2:C:71:LEU:N	0.50	2.72	4	1
1:A:593:HIS:N	1:A:593:HIS:ND1	0.50	2.59	4	3
1:A:510:LEU:HB3	1:A:511:PRO:HD3	0.50	1.83	2	4
2:C:73:LEU:N	2:C:73:LEU:HD12	0.50	2.21	3	1
1:A:532:HIS:C	1:A:532:HIS:HD1	0.50	2.15	4	1
2:B:58:ASP:C	2:B:59:TYR:CD1	0.50	2.90	7	3
1:A:515:SER:C	2:B:42:ARG:HH12	0.50	2.14	8	1
1:A:506:LEU:C	1:A:508:LEU:N	0.50	2.66	6	2
1:A:593:HIS:O	1:A:593:HIS:CG	0.50	2.64	1	1
2:C:73:LEU:O	2:C:74:ARG:C	0.50	2.55	6	3
1:A:549:ASN:C	1:A:549:ASN:HD22	0.50	2.15	7	2
2:B:25:ASN:C	2:B:25:ASN:HD22	0.50	2.15	1	2
1:A:552:GLU:OE2	2:C:72:ARG:NH1	0.50	2.45	2	1
2:B:60:ASN:N	2:B:60:ASN:OD1	0.50	2.45	4	1
2:C:20:SER:O	2:C:21:ASP:C	0.50	2.53	10	2
2:B:60:ASN:O	2:B:60:ASN:ND2	0.50	2.45	9	1
2:C:60:ASN:O	2:C:62:GLN:NE2	0.50	2.44	4	1
1:A:517:ASP:C	1:A:518:LEU:HD22	0.50	2.32	8	1
1:A:507:GLY:O	2:B:68:HIS:CD2	0.49	2.65	6	1
2:B:42:ARG:NE	2:B:49:GLN:OE1	0.49	2.45	9	2
1:A:575:MET:C	1:A:575:MET:SD	0.49	2.95	9	1
2:B:1:MET:N	2:B:17:VAL:O	0.49	2.38	6	4
2:C:52:ASP:OD1	2:C:52:ASP:N	0.49	2.45	9	5
2:B:20:SER:O	2:B:21:ASP:C	0.49	2.55	2	2
1:A:530:LEU:C	1:A:530:LEU:HD23	0.49	2.31	5	6
2:C:62:GLN:CD	2:C:62:GLN:H	0.49	2.14	4	1
2:B:15:LEU:N	2:B:15:LEU:HD12	0.49	2.22	10	2
2:C:15:LEU:HD12	2:C:15:LEU:N	0.49	2.22	8	1
2:C:55:THR:OG1	2:C:57:SER:OG	0.49	2.29	2	2
1:A:585:LEU:N	1:A:585:LEU:HD12	0.49	2.23	4	1
1:A:575:MET:SD	1:A:575:MET:O	0.49	2.70	9	1
1:A:532:HIS:C	1:A:532:HIS:ND1	0.49	2.70	4	1
1:A:507:GLY:O	2:B:68:HIS:NE2	0.49	2.46	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:43:LEU:N	2:B:43:LEU:CD1	0.49	2.75	7	1
2:B:25:ASN:ND2	2:B:29:LYS:HZ2	0.49	2.06	5	1
2:B:18:GLU:C	2:B:20:SER:H	0.49	2.15	4	2
1:A:511:PRO:C	1:A:513:ALA:N	0.49	2.70	7	6
2:C:54:ARG:NE	2:C:54:ARG:CA	0.49	2.75	3	1
2:B:32:ASP:N	2:B:32:ASP:OD1	0.49	2.46	6	1
1:A:506:LEU:HD12	1:A:506:LEU:N	0.49	2.23	2	2
2:C:55:THR:HG1	2:C:57:SER:HG	0.49	1.48	4	1
2:C:48:LYS:CD	2:C:49:GLN:H	0.49	2.20	8	1
1:A:551:LEU:C	1:A:553:ARG:N	0.48	2.71	1	1
1:A:535:VAL:HG13	1:A:536:GLY:N	0.48	2.23	4	4
2:B:48:LYS:NZ	2:C:75:GLY:O	0.48	2.47	3	2
2:C:18:GLU:O	2:C:21:ASP:N	0.48	2.46	5	3
2:B:22:THR:O	2:B:23:ILE:C	0.48	2.56	7	3
2:B:52:ASP:OD1	2:B:52:ASP:N	0.48	2.44	5	3
1:A:515:SER:OG	1:A:518:LEU:CD2	0.48	2.61	8	1
1:A:533:VAL:C	1:A:535:VAL:H	0.48	2.16	2	5
2:B:17:VAL:HG21	2:B:56:LEU:CD1	0.48	2.39	7	3
2:C:1:MET:N	2:C:17:VAL:O	0.48	2.37	9	6
1:A:515:SER:OG	1:A:518:LEU:HD12	0.48	2.07	3	1
1:A:511:PRO:C	1:A:513:ALA:H	0.48	2.17	7	2
1:A:523:ALA:O	1:A:524:ALA:C	0.48	2.55	3	1
1:A:592:GLU:N	1:A:592:GLU:CD	0.48	2.72	10	1
1:A:518:LEU:O	1:A:519:PRO:O	0.48	2.32	7	1
1:A:569:ALA:C	1:A:571:GLY:N	0.48	2.72	6	8
2:C:71:LEU:O	2:C:73:LEU:N	0.48	2.46	6	1
1:A:502:ASN:CG	1:A:503:ASP:H	0.48	2.17	2	3
1:A:568:LEU:C	1:A:568:LEU:HD23	0.48	2.34	6	2
2:B:69:LEU:HD23	2:B:70:VAL:N	0.48	2.24	5	1
1:A:571:GLY:C	1:A:573:LEU:N	0.48	2.71	10	5
1:A:512:ILE:HG22	1:A:512:ILE:O	0.48	2.09	7	2
1:A:550:PHE:CE1	1:A:566:LEU:HD21	0.48	2.43	10	2
1:A:562:TRP:C	1:A:564:ARG:N	0.47	2.71	3	2
2:C:62:GLN:CD	2:C:62:GLN:N	0.47	2.72	4	1
1:A:540:GLY:O	1:A:543:THR:N	0.47	2.48	6	1
1:A:553:ARG:NH1	1:A:562:TRP:CZ3	0.47	2.82	2	1
1:A:509:LEU:O	1:A:510:LEU:C	0.47	2.57	8	5
1:A:526:ALA:C	1:A:528:LEU:N	0.47	2.72	3	1
1:A:528:LEU:HD23	1:A:528:LEU:O	0.47	2.09	10	2
2:B:38:PRO:O	2:B:39:ASP:C	0.47	2.57	3	5
2:B:18:GLU:C	2:B:20:SER:N	0.47	2.70	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:50:LEU:CD2	2:B:59:TYR:CD2	0.47	2.98	3	1
1:A:510:LEU:N	1:A:511:PRO:HD2	0.47	2.24	4	8
1:A:515:SER:OG	1:A:518:LEU:CD1	0.47	2.62	3	1
2:C:7:THR:C	2:C:9:THR:H	0.47	2.17	6	2
2:B:57:SER:C	2:B:59:TYR:H	0.47	2.17	10	3
2:B:14:THR:C	2:B:15:LEU:HD12	0.47	2.34	4	3
1:A:551:LEU:N	1:A:551:LEU:HD12	0.47	2.23	8	3
1:A:596:THR:O	1:A:599:ILE:N	0.47	2.48	10	2
2:B:7:THR:C	2:B:9:THR:H	0.47	2.18	6	2
2:B:45:PHE:O	2:B:48:LYS:N	0.47	2.48	7	2
1:A:528:LEU:C	1:A:528:LEU:CD1	0.47	2.88	8	3
2:B:48:LYS:CB	2:B:48:LYS:NZ	0.47	2.78	4	1
2:B:71:LEU:HD12	2:B:71:LEU:N	0.47	2.25	6	1
2:B:49:GLN:NE2	2:B:50:LEU:O	0.47	2.47	10	1
2:B:18:GLU:O	2:B:21:ASP:N	0.46	2.46	6	4
2:B:42:ARG:CZ	2:B:49:GLN:OE1	0.46	2.63	5	1
2:C:31:GLN:OE1	2:C:36:ILE:C	0.46	2.58	9	1
1:A:510:LEU:O	1:A:514:ALA:CB	0.46	2.63	10	1
2:B:53:GLY:O	2:B:54:ARG:O	0.46	2.32	6	8
2:B:59:TYR:O	2:B:60:ASN:CG	0.46	2.58	8	1
1:A:496:ALA:O	1:A:498:ALA:N	0.46	2.49	2	1
1:A:515:SER:C	1:A:516:THR:OG1	0.46	2.59	8	4
1:A:538:CYS:C	1:A:539:ASN:ND2	0.46	2.73	8	1
2:C:17:VAL:C	2:C:18:GLU:CD	0.46	2.84	9	1
1:A:543:THR:O	1:A:544:THR:C	0.46	2.59	8	4
1:A:593:HIS:O	1:A:595:MET:SD	0.46	2.74	10	1
2:B:49:GLN:CD	2:B:49:GLN:C	0.46	2.84	3	2
1:A:528:LEU:C	1:A:528:LEU:HD23	0.46	2.35	6	2
1:A:566:LEU:N	1:A:566:LEU:CD1	0.46	2.78	5	1
1:A:568:LEU:C	1:A:568:LEU:CD1	0.46	2.89	2	1
1:A:528:LEU:C	1:A:528:LEU:HD13	0.46	2.36	8	3
1:A:591:ILE:O	1:A:592:GLU:O	0.46	2.33	3	4
1:A:507:GLY:C	1:A:508:LEU:HD12	0.46	2.36	7	2
1:A:537:THR:O	1:A:538:CYS:C	0.46	2.59	3	1
1:A:548:ASP:OD1	2:C:42:ARG:NH2	0.45	2.49	8	1
1:A:602:LEU:CD1	1:A:602:LEU:C	0.45	2.89	9	1
2:B:22:THR:OG1	2:B:24:GLU:CG	0.45	2.64	9	1
1:A:550:PHE:CE1	1:A:553:ARG:NH1	0.45	2.84	1	1
1:A:594:PRO:C	1:A:596:THR:H	0.45	2.18	1	1
2:C:53:GLY:O	2:C:54:ARG:O	0.45	2.32	2	7
1:A:565:PHE:O	1:A:568:LEU:N	0.45	2.48	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:510:LEU:HD11	1:A:545:SER:OG	0.45	2.11	10	1
1:A:592:GLU:O	1:A:593:HIS:CG	0.45	2.69	2	1
2:B:39:ASP:C	2:B:40:GLN:NE2	0.45	2.74	9	2
1:A:568:LEU:C	1:A:568:LEU:HD13	0.45	2.37	2	1
1:A:572:ILE:C	1:A:574:TYR:N	0.45	2.74	4	1
1:A:590:ALA:O	2:C:47:GLY:O	0.45	2.33	4	1
1:A:565:PHE:O	1:A:568:LEU:CB	0.45	2.64	6	1
1:A:537:THR:O	1:A:537:THR:HG23	0.45	2.12	2	2
1:A:551:LEU:C	1:A:553:ARG:H	0.45	2.19	7	3
1:A:549:ASN:C	1:A:549:ASN:ND2	0.45	2.74	3	1
2:C:63:LYS:CB	2:C:63:LYS:NZ	0.45	2.80	5	1
1:A:602:LEU:C	1:A:602:LEU:HD13	0.45	2.37	9	1
2:B:70:VAL:C	2:B:71:LEU:HD22	0.45	2.36	9	1
2:C:53:GLY:O	2:C:54:ARG:C	0.45	2.60	1	2
2:C:59:TYR:O	2:C:60:ASN:CG	0.45	2.60	4	2
1:A:497:PHE:O	1:A:498:ALA:C	0.45	2.59	6	3
1:A:504:GLU:OE2	2:B:6:LYS:NZ	0.45	2.50	5	1
2:B:38:PRO:O	2:B:41:GLN:N	0.45	2.50	10	1
1:A:496:ALA:C	1:A:498:ALA:N	0.45	2.71	2	1
1:A:522:THR:C	1:A:524:ALA:N	0.45	2.74	2	2
2:B:45:PHE:O	2:B:46:ALA:HB3	0.45	2.12	4	1
2:C:24:GLU:CD	2:C:24:GLU:C	0.45	2.85	7	1
2:C:16:GLU:CD	2:C:16:GLU:H	0.45	2.20	1	2
1:A:526:ALA:O	1:A:528:LEU:N	0.45	2.50	3	1
2:B:22:THR:O	2:B:25:ASN:N	0.45	2.50	7	3
1:A:600:GLU:CD	1:A:600:GLU:C	0.45	2.85	4	2
2:C:18:GLU:CB	2:C:19:PRO:CD	0.45	2.95	7	3
1:A:550:PHE:CZ	1:A:553:ARG:NH1	0.45	2.85	1	1
2:C:55:THR:C	2:C:57:SER:H	0.44	2.20	1	1
1:A:517:ASP:C	2:B:72:ARG:HH21	0.44	2.20	3	1
1:A:569:ALA:O	1:A:571:GLY:N	0.44	2.50	6	3
1:A:495:ILE:HG22	1:A:495:ILE:O	0.44	2.12	6	2
1:A:522:THR:O	1:A:523:ALA:C	0.44	2.61	2	2
2:C:50:LEU:CD2	2:C:59:TYR:CD2	0.44	3.00	2	1
1:A:545:SER:OG	1:A:546:ILE:N	0.44	2.49	3	1
2:B:42:ARG:NH1	2:B:49:GLN:CD	0.44	2.75	5	1
1:A:587:THR:O	1:A:590:ALA:N	0.44	2.50	10	5
1:A:520:ILE:O	1:A:520:ILE:HG22	0.44	2.11	2	1
1:A:530:LEU:C	1:A:530:LEU:CD2	0.44	2.90	5	4
1:A:536:GLY:O	1:A:537:THR:O	0.44	2.34	3	1
1:A:494:GLY:C	1:A:496:ALA:N	0.44	2.74	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:552:GLU:C	1:A:553:ARG:O	0.44	2.60	5	1
1:A:585:LEU:O	1:A:586:GLU:C	0.44	2.60	5	1
1:A:538:CYS:C	1:A:539:ASN:OD1	0.44	2.60	2	1
2:B:72:ARG:CD	2:B:72:ARG:C	0.44	2.90	3	1
1:A:569:ALA:C	1:A:571:GLY:H	0.44	2.20	9	2
2:C:73:LEU:C	2:C:73:LEU:HD13	0.44	2.37	7	1
1:A:568:LEU:O	1:A:571:GLY:N	0.44	2.50	10	1
2:C:73:LEU:C	2:C:73:LEU:CD1	0.44	2.90	7	1
2:C:15:LEU:N	2:C:15:LEU:CD1	0.44	2.81	8	1
1:A:535:VAL:CG1	1:A:536:GLY:N	0.44	2.81	4	2
1:A:539:ASN:CG	1:A:539:ASN:O	0.44	2.61	3	1
2:B:58:ASP:OD1	2:B:58:ASP:N	0.44	2.51	9	1
2:C:38:PRO:O	2:C:39:ASP:C	0.44	2.61	2	3
1:A:591:ILE:O	1:A:592:GLU:C	0.44	2.61	4	1
1:A:561:ASP:O	1:A:561:ASP:OD1	0.44	2.36	5	2
2:C:73:LEU:O	2:C:74:ARG:O	0.44	2.36	6	3
2:C:31:GLN:OE1	2:C:36:ILE:O	0.44	2.35	9	1
1:A:568:LEU:C	1:A:568:LEU:CD2	0.44	2.91	3	2
1:A:544:THR:O	1:A:548:ASP:OD1	0.44	2.36	4	1
2:B:15:LEU:N	2:B:15:LEU:CD1	0.44	2.81	4	2
1:A:520:ILE:O	1:A:521:GLU:O	0.44	2.35	7	1
1:A:497:PHE:O	1:A:499:GLY:N	0.44	2.50	10	1
1:A:549:ASN:O	1:A:553:ARG:N	0.43	2.48	3	1
1:A:528:LEU:C	1:A:528:LEU:CD2	0.43	2.91	5	2
1:A:571:GLY:C	1:A:573:LEU:H	0.43	2.20	10	1
2:C:27:LYS:NZ	2:C:41:GLN:O	0.43	2.43	10	1
1:A:515:SER:OG	1:A:518:LEU:HD23	0.43	2.13	8	1
2:B:24:GLU:CD	2:B:24:GLU:C	0.43	2.85	10	1
1:A:531:ALA:O	1:A:535:VAL:N	0.43	2.51	4	5
1:A:553:ARG:HH12	1:A:595:MET:CG	0.43	2.26	4	1
2:B:71:LEU:O	2:B:72:ARG:CB	0.43	2.64	5	1
2:B:25:ASN:O	2:B:28:ALA:HB3	0.43	2.13	7	1
2:C:60:ASN:OD1	2:C:60:ASN:O	0.43	2.36	7	1
1:A:602:LEU:C	1:A:604:GLY:N	0.43	2.75	8	1
1:A:562:TRP:O	1:A:564:ARG:N	0.43	2.51	3	1
2:B:31:GLN:O	2:B:31:GLN:OE1	0.43	2.37	4	1
1:A:548:ASP:O	1:A:552:GLU:OE2	0.43	2.37	8	1
2:C:22:THR:O	2:C:23:ILE:C	0.43	2.61	5	1
1:A:592:GLU:CD	1:A:592:GLU:N	0.43	2.75	8	1
2:B:59:TYR:C	2:B:60:ASN:CG	0.43	2.86	8	1
1:A:529:ALA:O	1:A:533:VAL:HG23	0.43	2.14	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:594:PRO:C	1:A:596:THR:N	0.43	2.77	1	1
1:A:595:MET:C	1:A:597:SER:H	0.43	2.21	7	3
1:A:538:CYS:O	1:A:539:ASN:CG	0.43	2.62	6	4
1:A:561:ASP:C	1:A:562:TRP:CG	0.43	2.97	8	1
1:A:563:VAL:O	1:A:563:VAL:HG22	0.43	2.13	8	2
1:A:522:THR:O	1:A:524:ALA:N	0.43	2.52	2	2
1:A:572:ILE:O	1:A:573:LEU:C	0.43	2.62	5	1
2:B:55:THR:OG1	2:B:57:SER:OG	0.43	2.36	6	1
2:C:14:THR:C	2:C:15:LEU:HD12	0.43	2.38	8	1
2:C:25:ASN:ND2	2:C:29:LYS:HZ2	0.43	2.10	1	1
1:A:495:ILE:O	1:A:495:ILE:HG22	0.43	2.14	5	1
2:B:18:GLU:CB	2:B:19:PRO:CD	0.43	2.97	8	2
1:A:506:LEU:C	1:A:508:LEU:H	0.43	2.20	6	1
1:A:531:ALA:O	1:A:532:HIS:C	0.43	2.61	3	2
2:B:32:ASP:OD1	2:B:32:ASP:C	0.43	2.62	4	1
1:A:506:LEU:CD2	1:A:530:LEU:HD22	0.43	2.43	9	1
2:B:71:LEU:O	2:B:72:ARG:C	0.42	2.62	6	1
1:A:494:GLY:C	1:A:496:ALA:H	0.42	2.22	4	1
2:C:55:THR:C	2:C:57:SER:N	0.42	2.77	1	1
1:A:606:CYS:O	1:A:607:ALA:HB2	0.42	2.14	5	1
1:A:593:HIS:CD2	1:A:593:HIS:N	0.42	2.87	10	1
1:A:532:HIS:ND1	1:A:532:HIS:O	0.42	2.51	4	2
2:C:46:ALA:C	2:C:48:LYS:H	0.42	2.22	4	1
1:A:579:GLU:O	1:A:580:GLN:C	0.42	2.62	5	1
2:B:42:ARG:CZ	2:B:49:GLN:CD	0.42	2.93	5	1
2:B:59:TYR:C	2:B:60:ASN:OD1	0.42	2.62	8	1
2:C:57:SER:C	2:C:59:TYR:N	0.42	2.76	8	1
2:B:8:LEU:C	2:B:9:THR:HG1	0.42	2.22	9	1
1:A:568:LEU:O	1:A:569:ALA:C	0.42	2.62	10	1
2:C:18:GLU:C	2:C:20:SER:N	0.42	2.78	5	2
2:B:49:GLN:OE1	2:B:50:LEU:O	0.42	2.37	3	1
1:A:515:SER:OG	1:A:518:LEU:HD11	0.42	2.15	4	1
1:A:502:ASN:C	1:A:504:GLU:N	0.42	2.77	6	1
1:A:563:VAL:HG13	1:A:564:ARG:N	0.42	2.28	6	1
1:A:561:ASP:C	1:A:562:TRP:CD1	0.42	2.98	8	1
2:B:49:GLN:C	2:B:49:GLN:OE1	0.42	2.63	10	1
1:A:579:GLU:O	1:A:582:ASP:N	0.42	2.51	5	1
2:B:4:PHE:CE2	2:B:14:THR:OG1	0.42	2.61	6	1
2:C:71:LEU:O	2:C:72:ARG:C	0.42	2.62	2	1
2:B:21:ASP:OD1	2:B:21:ASP:N	0.42	2.52	4	1
1:A:551:LEU:N	1:A:551:LEU:CD1	0.42	2.82	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:512:ILE:O	1:A:512:ILE:HG22	0.42	2.15	10	2
1:A:553:ARG:NH1	1:A:595:MET:SD	0.42	2.93	4	1
1:A:587:THR:O	1:A:590:ALA:HB3	0.42	2.15	5	1
1:A:510:LEU:CD2	2:C:74:ARG:HE	0.42	2.28	7	1
1:A:510:LEU:O	1:A:513:ALA:C	0.42	2.62	10	1
2:C:32:ASP:OD1	2:C:32:ASP:C	0.42	2.62	2	1
1:A:539:ASN:O	1:A:539:ASN:OD1	0.42	2.38	3	1
1:A:517:ASP:O	1:A:517:ASP:OD1	0.42	2.37	7	1
1:A:568:LEU:HD12	1:A:568:LEU:N	0.42	2.30	9	1
1:A:501:LYS:NZ	1:A:537:THR:HG21	0.42	2.30	3	1
1:A:603:VAL:O	1:A:606:CYS:O	0.42	2.38	5	1
2:C:22:THR:O	2:C:25:ASN:N	0.42	2.53	5	1
1:A:544:THR:O	1:A:548:ASP:OD2	0.41	2.38	5	3
2:B:42:ARG:NE	2:B:72:ARG:O	0.41	2.53	3	1
2:B:15:LEU:HD12	2:B:15:LEU:N	0.41	2.30	4	1
2:B:58:ASP:O	2:B:59:TYR:CG	0.41	2.73	7	1
1:A:496:ALA:O	1:A:497:PHE:C	0.41	2.63	1	2
1:A:502:ASN:C	1:A:504:GLU:H	0.41	2.22	6	2
2:C:66:THR:C	2:C:67:LEU:HD12	0.41	2.40	4	1
2:C:47:GLY:O	2:C:48:LYS:C	0.41	2.64	7	1
1:A:506:LEU:O	1:A:507:GLY:C	0.41	2.63	10	1
1:A:510:LEU:O	1:A:514:ALA:HB3	0.41	2.15	10	1
1:A:567:ALA:O	1:A:568:LEU:C	0.41	2.63	10	1
2:B:53:GLY:O	2:B:54:ARG:C	0.41	2.63	1	1
1:A:531:ALA:C	1:A:533:VAL:N	0.41	2.76	3	1
1:A:592:GLU:O	1:A:593:HIS:C	0.41	2.64	3	1
1:A:600:GLU:O	1:A:600:GLU:OE2	0.41	2.38	4	1
2:B:17:VAL:HG21	2:B:56:LEU:HD13	0.41	1.92	4	1
2:B:40:GLN:O	2:B:41:GLN:CG	0.41	2.68	8	1
1:A:523:ALA:O	1:A:527:SER:OG	0.41	2.38	2	1
1:A:549:ASN:ND2	1:A:549:ASN:O	0.41	2.52	3	1
2:B:71:LEU:N	2:B:71:LEU:CD1	0.41	2.84	6	1
2:B:58:ASP:N	2:B:58:ASP:OD1	0.41	2.51	7	1
2:C:59:TYR:O	2:C:60:ASN:CB	0.41	2.67	1	1
1:A:587:THR:OG1	2:C:68:HIS:CE1	0.41	2.73	10	1
2:B:18:GLU:N	2:B:21:ASP:OD1	0.41	2.53	10	1
1:A:540:GLY:O	1:A:541:ASP:C	0.41	2.63	2	2
1:A:596:THR:C	1:A:598:ALA:N	0.41	2.75	3	4
1:A:545:SER:OG	2:C:73:LEU:CD1	0.41	2.69	5	1
2:B:67:LEU:N	2:B:67:LEU:HD12	0.41	2.30	5	1
1:A:569:ALA:O	1:A:570:LEU:C	0.41	2.62	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:528:LEU:HD13	1:A:528:LEU:O	0.41	2.16	7	1
1:A:562:TRP:CD1	1:A:562:TRP:N	0.41	2.89	4	1
1:A:562:TRP:O	1:A:563:VAL:C	0.41	2.63	6	1
2:B:42:ARG:HE	2:B:49:GLN:CG	0.41	2.29	6	1
1:A:595:MET:SD	1:A:595:MET:N	0.41	2.93	10	1
2:B:28:ALA:O	2:B:32:ASP:OD1	0.41	2.37	6	1
2:C:45:PHE:C	2:C:47:GLY:H	0.41	2.24	7	1
2:B:8:LEU:C	2:B:9:THR:OG1	0.41	2.64	9	1
2:B:18:GLU:O	2:B:21:ASP:OD1	0.41	2.39	9	1
2:B:32:ASP:OD1	2:B:32:ASP:N	0.41	2.53	9	1
1:A:583:ASP:O	1:A:584:VAL:C	0.41	2.64	10	1
1:A:531:ALA:O	1:A:533:VAL:N	0.41	2.54	3	1
2:C:71:LEU:CD1	2:C:71:LEU:C	0.41	2.94	3	1
1:A:595:MET:O	1:A:596:THR:C	0.41	2.64	7	1
1:A:516:THR:O	1:A:552:GLU:OE1	0.41	2.39	10	1
2:C:18:GLU:O	2:C:20:SER:N	0.40	2.55	5	1
2:B:7:THR:C	2:B:9:THR:N	0.40	2.79	6	1
1:A:550:PHE:O	1:A:551:LEU:C	0.40	2.64	7	1
1:A:580:GLN:CG	1:A:581:VAL:N	0.40	2.84	10	1
2:C:17:VAL:HG21	2:C:56:LEU:CD1	0.40	2.46	2	1
2:C:53:GLY:C	2:C:54:ARG:O	0.40	2.65	2	1
1:A:526:ALA:O	1:A:527:SER:C	0.40	2.62	3	1
2:C:71:LEU:HD12	2:C:71:LEU:C	0.40	2.41	3	1
1:A:519:PRO:C	1:A:521:GLU:H	0.40	2.24	5	1
1:A:506:LEU:N	1:A:506:LEU:CD1	0.40	2.84	7	1
1:A:541:ASP:O	1:A:542:ILE:C	0.40	2.65	7	1
1:A:530:LEU:HD23	1:A:530:LEU:O	0.40	2.16	8	1
2:B:45:PHE:C	2:B:47:GLY:N	0.40	2.79	2	1
2:C:59:TYR:O	2:C:60:ASN:C	0.40	2.64	7	2
2:B:60:ASN:ND2	2:B:60:ASN:N	0.40	2.67	5	1
2:C:5:VAL:N	2:C:13:ILE:O	0.40	2.54	8	1
2:C:57:SER:C	2:C:59:TYR:H	0.40	2.23	10	1
1:A:546:ILE:O	1:A:550:PHE:CD1	0.40	2.74	2	1
1:A:568:LEU:N	1:A:568:LEU:CD1	0.40	2.85	9	1
1:A:585:LEU:N	1:A:585:LEU:CD1	0.40	2.85	4	1
2:C:49:GLN:O	2:C:51:GLU:OE2	0.40	2.39	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	104/131 (79%)	65±6 (62±6%)	29±6 (28±6%)	10±2 (10±2%)	1	10
2	B	71/76 (93%)	55±3 (78±4%)	12±2 (17±3%)	4±1 (5±1%)	2	22
2	C	74/76 (97%)	56±2 (76±2%)	12±2 (16±3%)	6±1 (8±1%)	1	14
All	All	2490/2830 (88%)	1759 (71%)	533 (21%)	198 (8%)	1	13

All 57 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	516	THR	10
2	B	35	GLY	10
2	C	35	GLY	10
2	C	54	ARG	10
2	B	54	ARG	9
1	A	562	TRP	8
2	C	46	ALA	8
2	B	39	ASP	7
2	C	10	GLY	7
1	A	607	ALA	6
2	C	74	ARG	6
1	A	500	SER	5
1	A	518	LEU	5
1	A	592	GLU	5
1	A	553	ARG	5
1	A	521	GLU	4
1	A	575	MET	4
1	A	602	LEU	4
2	C	39	ASP	4
1	A	519	PRO	4
1	A	537	THR	4
1	A	579	GLU	3
1	A	594	PRO	3
2	C	47	GLY	3
1	A	561	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	573	LEU	3
1	A	514	ALA	3
2	C	73	LEU	3
2	C	48	LYS	3
1	A	497	PHE	2
1	A	501	LYS	2
2	B	34	GLU	2
1	A	569	ALA	2
1	A	517	ASP	2
2	B	10	GLY	2
2	B	19	PRO	2
1	A	515	SER	2
1	A	570	LEU	2
2	B	7	THR	2
1	A	552	GLU	2
1	A	499	GLY	1
1	A	533	VAL	1
2	B	52	ASP	1
1	A	534	PHE	1
2	B	61	ILE	1
2	C	75	GLY	1
1	A	527	SER	1
2	C	9	THR	1
1	A	507	GLY	1
2	C	72	ARG	1
1	A	505	VAL	1
1	A	596	THR	1
2	B	72	ARG	1
1	A	498	ALA	1
1	A	503	ASP	1
2	B	9	THR	1
2	C	34	GLU	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	83/102 (81%)	80±2 (96±2%)	3±2 (4±2%)	29 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	66/68 (97%)	62±1 (94±2%)	4±1 (6±2%)	18 67
2	C	68/68 (100%)	64±1 (93±2%)	4±1 (7±2%)	17 66
All	All	2170/2380 (91%)	2050 (94%)	120 (6%)	21 71

All 37 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	546	ILE	10
2	B	52	ASP	10
2	C	52	ASP	10
2	B	20	SER	8
2	C	8	LEU	7
2	C	20	SER	7
2	B	8	LEU	5
1	A	528	LEU	5
2	B	70	VAL	5
2	B	13	ILE	4
2	C	1	MET	4
2	B	1	MET	3
1	A	537	THR	3
2	C	71	LEU	3
1	A	510	LEU	3
2	B	25	ASN	3
2	C	73	LEU	3
2	C	25	ASN	2
1	A	505	VAL	2
1	A	552	GLU	2
2	B	60	ASN	2
2	C	68	HIS	2
1	A	516	THR	2
2	C	18	GLU	2
1	A	568	LEU	1
1	A	535	VAL	1
1	A	545	SER	1
2	B	48	LYS	1
2	C	63	LYS	1
1	A	549	ASN	1
2	C	13	ILE	1
2	C	48	LYS	1
1	A	602	LEU	1

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Mol	Chain	Res	Type	Models (Total)
2	B	9	THR	1
2	C	44	ILE	1
1	A	595	MET	1
2	C	67	LEU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 27% for the well-defined parts and 27% 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	1034
Number of shifts mapped to atoms	1034
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
$^{13}\text{C}_\alpha$	96	-0.46 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	92	0.23 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	63	0.81 ± 0.56	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 27%, i.e. 912 atoms were assigned a chemical shift out of a possible 3437. 0 out of 47 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	294/1259 (23%)	150/512 (29%)	86/504 (17%)	58/243 (24%)
Sidechain	598/2031 (29%)	417/1329 (31%)	181/640 (28%)	0/62 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	20/147 (14%)	20/74 (27%)	0/68 (0%)	0/5 (0%)
Overall	912/3437 (27%)	587/1915 (31%)	267/1212 (22%)	58/310 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 27%, i.e. 1034 atoms were assigned a chemical shift out of a possible 3815. 0 out of 51 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	324/1421 (23%)	165/581 (28%)	96/566 (17%)	63/274 (23%)
Sidechain	686/2238 (31%)	478/1466 (33%)	208/704 (30%)	0/68 (0%)
Aromatic	24/156 (15%)	24/78 (31%)	0/73 (0%)	0/5 (0%)
Overall	1034/3815 (27%)	667/2125 (31%)	304/1343 (23%)	63/347 (18%)

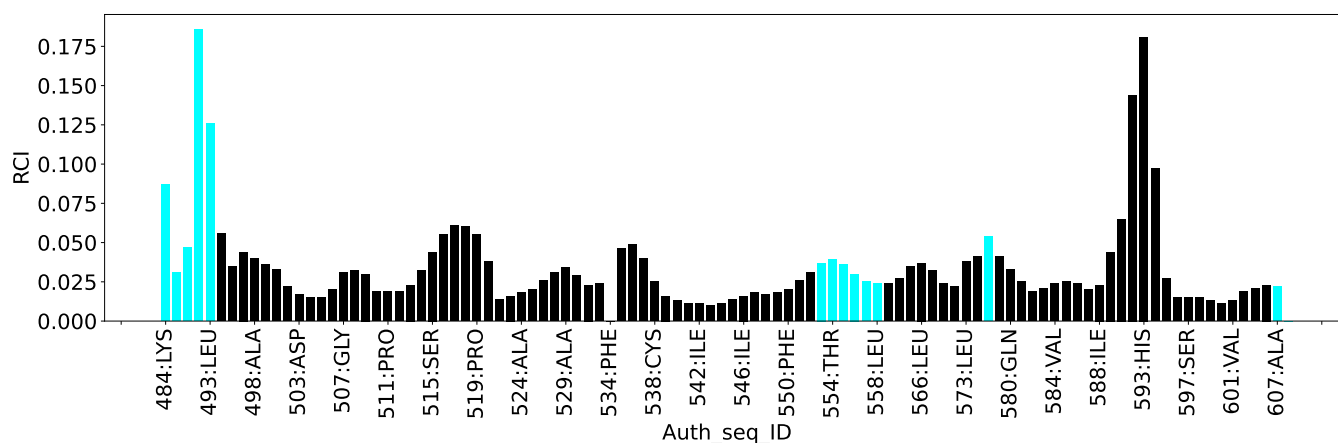
7.1.4 Statistically unusual chemical shifts [i](#)

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	6377
Intra-residue ($ i-j =0$)	1692
Sequential ($ i-j =1$)	980
Medium range ($ i-j >1$ and $ i-j <5$)	1029
Long range ($ i-j \geq 5$)	2381
Inter-chain	115
Hydrogen bond restraints	180
Disulfide bond restraints	0
Total dihedral-angle restraints	249
Number of unmapped restraints	0
Number of restraints per residue	23.4
Number of long range restraints per residue ¹	8.5

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)	16.5	0.2
0.2-0.5 (Medium)	30.7	0.5
>0.5 (Large)	153.3	33.23

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	3.9	8.56
10.0-20.0 (Medium)	0.1	14.63
>20.0 (Large)	0.6	74.03

9 Distance violation analysis ⓘ

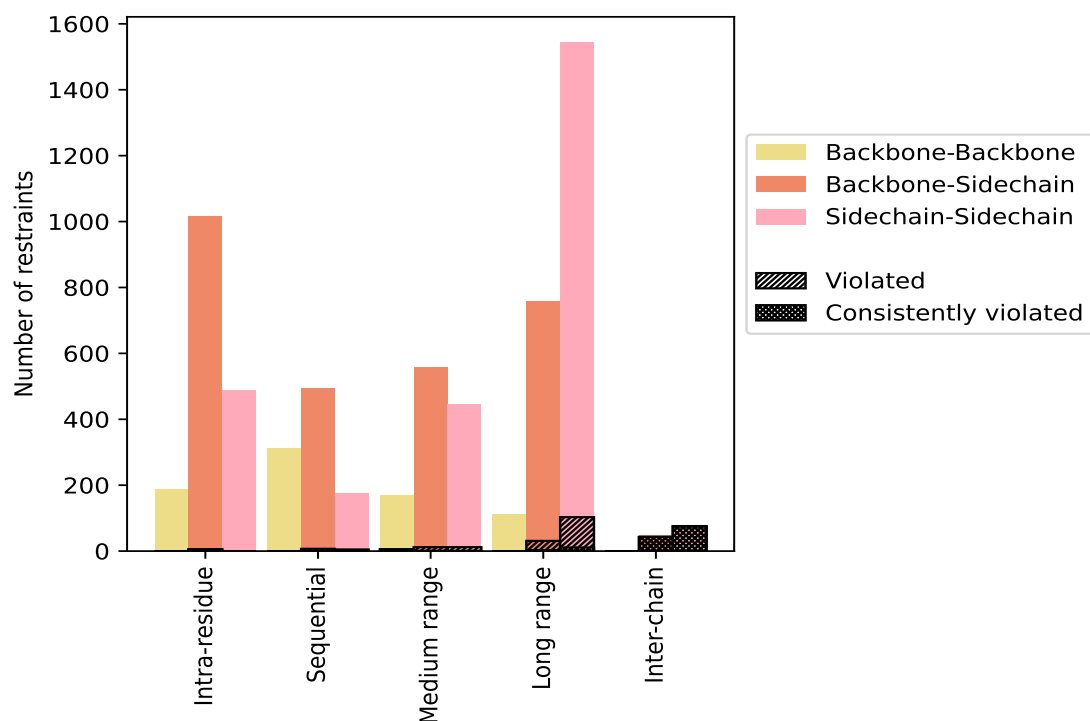
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1692	26.5	6	0.4	0.1	4	0.2	0.1
Backbone-Backbone	188	2.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1016	15.9	6	0.6	0.1	4	0.4	0.1
Sidechain-Sidechain	488	7.7	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	980	15.4	12	1.2	0.2	0	0.0	0.0
Backbone-Backbone	311	4.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	495	7.8	7	1.4	0.1	0	0.0	0.0
Sidechain-Sidechain	174	2.7	5	2.9	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	1029	16.1	28	2.7	0.4	4	0.4	0.1
Backbone-Backbone	168	2.6	6	3.6	0.1	2	1.2	0.0
Backbone-Sidechain	416	6.5	10	2.4	0.2	1	0.2	0.0
Sidechain-Sidechain	445	7.0	12	2.7	0.2	1	0.2	0.0
Long range ($i-j \geq 5$)	2381	37.3	134	5.6	2.1	14	0.6	0.2
Backbone-Backbone	112	1.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	725	11.4	31	4.3	0.5	3	0.4	0.0
Sidechain-Sidechain	1544	24.2	103	6.7	1.6	11	0.7	0.2
Inter-chain	115	1.8	111	96.5	1.7	109	94.8	1.7
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	47	0.7	43	91.5	0.7	43	91.5	0.7
Sidechain-Sidechain	68	1.1	68	100.0	1.1	66	97.1	1.0
Hydrogen bond	180	2.8	10	5.6	0.2	8	4.4	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	6377	100.0	301	4.7	4.7	139	2.2	2.2
Backbone-Backbone	779	12.2	6	0.8	0.1	2	0.3	0.0
Backbone-Sidechain	2871	45.0	99	3.4	1.6	51	1.8	0.8
Sidechain-Sidechain	2727	42.8	196	7.2	3.1	86	3.2	1.3

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

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



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

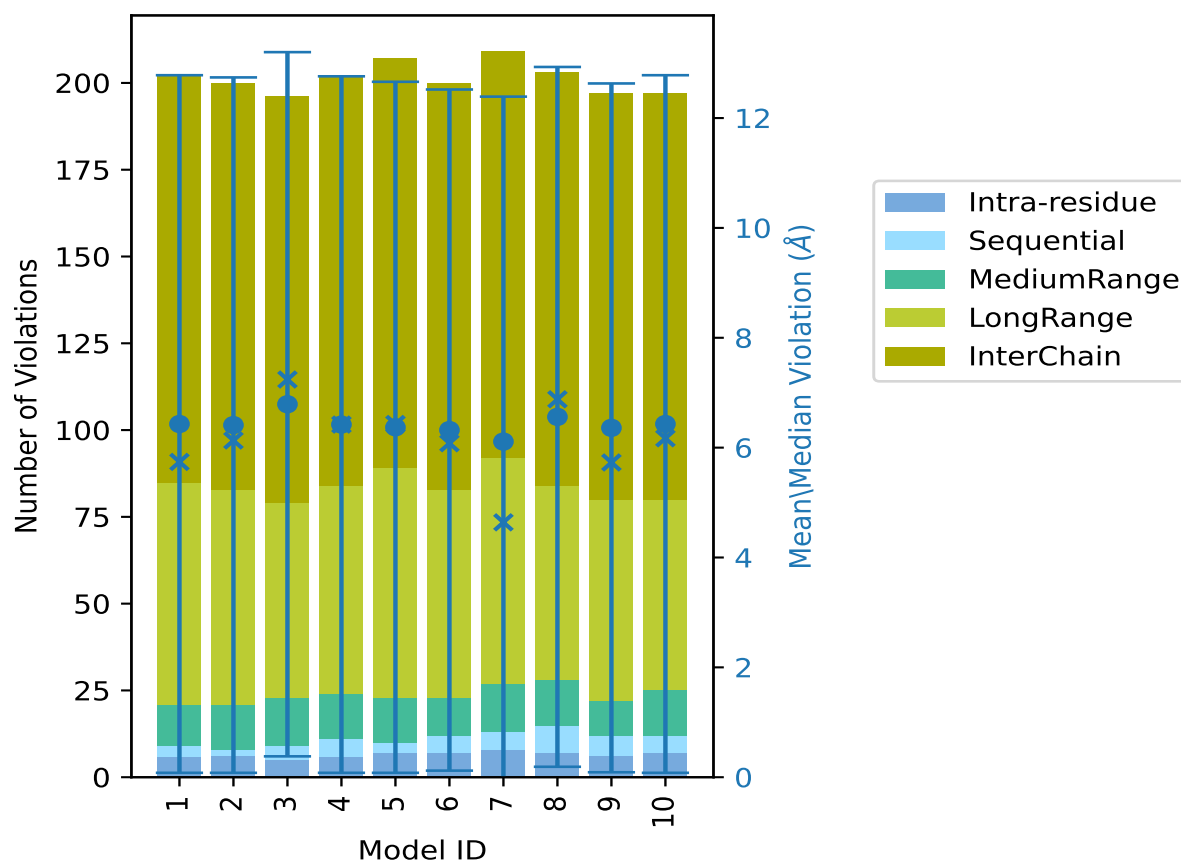
9.2 Distance violation statistics for each model [i](#)

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	6	3	12	64	117	202	6.43	30.18	6.35	5.74
2	6	2	13	62	117	200	6.41	30.94	6.33	6.13
3	5	4	14	56	117	196	6.79	30.56	6.41	7.24
4	6	5	13	60	118	202	6.42	32.81	6.34	6.42
5	7	3	13	66	118	207	6.37	28.56	6.29	6.43
6	7	5	11	60	117	200	6.32	33.23	6.2	6.08
7	8	5	14	65	117	209	6.11	31.26	6.28	4.64
8	7	8	13	56	119	203	6.56	30.21	6.37	6.88
9	6	6	10	58	117	197	6.36	30.71	6.27	5.73
10	7	5	13	55	117	197	6.43	31.87	6.35	6.17

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 5906(IR:1686, SQ:968, MR:1001, LR:2247, IC:4) 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	%
1	5	6	33	0	45	1	10.0
0	0	5	12	2	19	2	20.0
0	2	3	17	0	22	3	30.0

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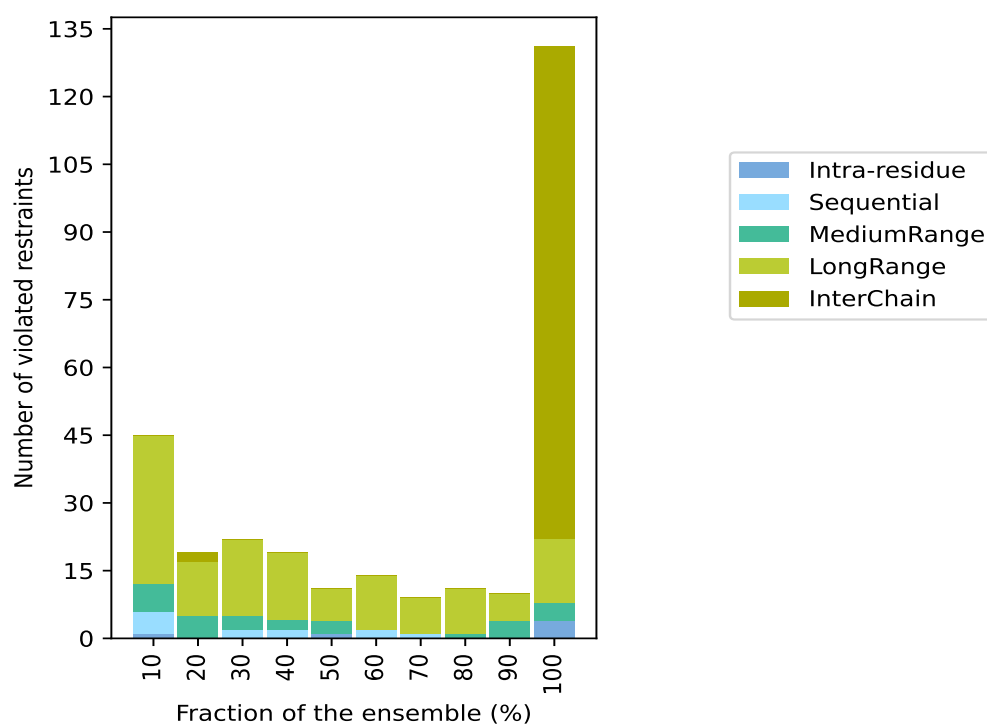
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	2	2	15	0	19	4	40.0
1	0	3	7	0	11	5	50.0
0	2	0	12	0	14	6	60.0
0	1	0	8	0	9	7	70.0
0	0	1	10	0	11	8	80.0
0	0	4	6	0	10	9	90.0
4	0	4	14	109	131	10	100.0

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

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

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

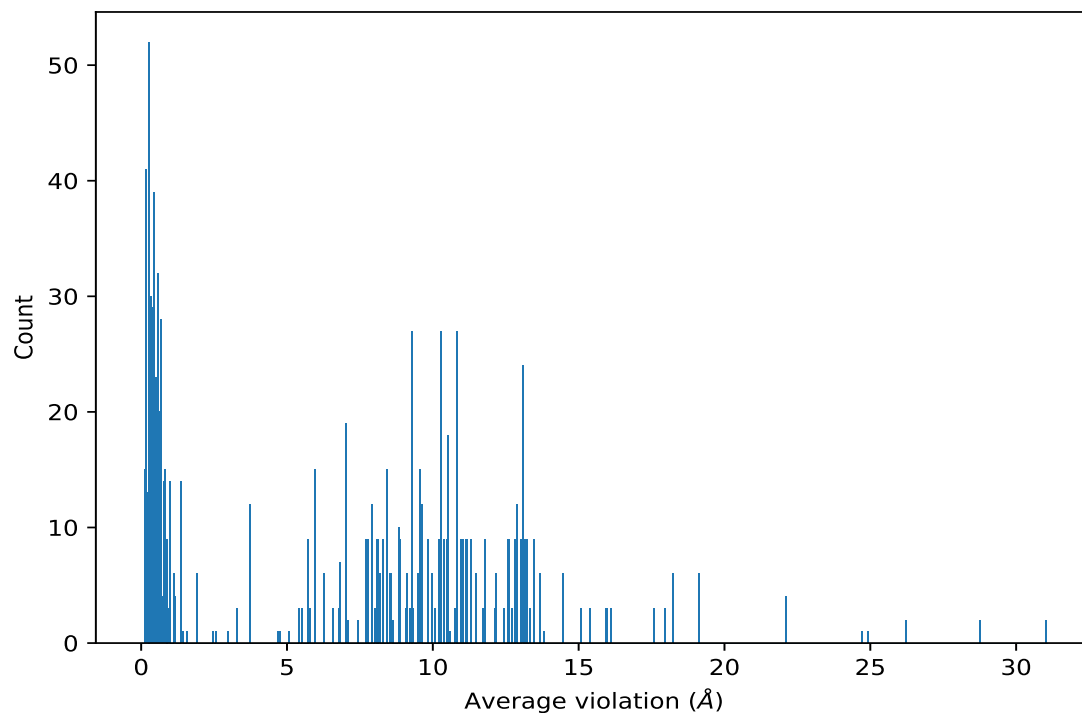


9.4 Most violated distance restraints in the ensemble [i](#)

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)
(1,102)	1:504:A:GLU:OE2	2:6:C:LYS:NZ	10	31.03	1.29	30.83
(1,102)	1:504:A:GLU:OE1	2:6:C:LYS:NZ	10	31.03	1.29	30.83
(1,66)	1:583:A:ASP:OD1	2:6:B:LYS:NZ	10	28.79	0.95	28.93
(1,66)	1:583:A:ASP:OD2	2:6:B:LYS:NZ	10	28.79	0.95	28.93
(1,67)	1:592:A:GLU:OE2	2:48:B:LYS:NZ	10	26.24	1.44	26.28
(1,67)	1:592:A:GLU:OE1	2:48:B:LYS:NZ	10	26.24	1.44	26.28
(2,1)	1:583:A:ASP:OD1	2:68:B:HIS:NE2	10	24.95	1.24	24.78
(2,2)	1:583:A:ASP:OD2	2:68:B:HIS:NE2	10	24.73	0.81	25.04
(1,63)	1:541:A:ASP:OD2	2:74:B:ARG:NH1	10	22.1	2.46	21.43
(1,63)	1:541:A:ASP:OD2	2:74:B:ARG:NH2	10	22.1	2.46	21.43
(1,63)	1:541:A:ASP:OD1	2:74:B:ARG:NH2	10	22.1	2.46	21.43
(1,63)	1:541:A:ASP:OD1	2:74:B:ARG:NH1	10	22.1	2.46	21.43
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD2	10	19.11	0.57	18.97
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD3	10	19.11	0.57	18.97
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD2	10	19.11	0.57	18.97

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD3	10	19.11	0.57	18.97
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD2	10	19.11	0.57	18.97
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD3	10	19.11	0.57	18.97
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD2	10	18.23	0.7	18.3
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD3	10	18.23	0.7	18.3
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD2	10	18.23	0.7	18.3
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD3	10	18.23	0.7	18.3
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD2	10	18.23	0.7	18.3
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD3	10	18.23	0.7	18.3
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG21	10	17.96	0.46	18.03
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG22	10	17.96	0.46	18.03
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG23	10	17.96	0.46	18.03
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD11	10	17.55	0.51	17.71
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD12	10	17.55	0.51	17.71
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD13	10	17.55	0.51	17.71
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG21	10	16.1	0.66	16.21
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG22	10	16.1	0.66	16.21
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG23	10	16.1	0.66	16.21
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG21	10	15.99	0.35	15.92
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG22	10	15.99	0.35	15.92
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG23	10	15.99	0.35	15.92
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG21	10	15.91	0.32	15.92
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG22	10	15.91	0.32	15.92
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG23	10	15.91	0.32	15.92
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD11	10	15.39	0.75	15.56
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD12	10	15.39	0.75	15.56
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD13	10	15.39	0.75	15.56
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD11	10	15.06	0.35	15.15
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD12	10	15.06	0.35	15.15
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD13	10	15.06	0.35	15.15
(1,74)	1:508:A:LEU:HD11	2:8:C:LEU:HG	10	14.48	0.66	14.7
(1,74)	1:508:A:LEU:HD12	2:8:C:LEU:HG	10	14.48	0.66	14.7
(1,74)	1:508:A:LEU:HD13	2:8:C:LEU:HG	10	14.48	0.66	14.7
(1,74)	1:508:A:LEU:HD21	2:8:C:LEU:HG	10	14.48	0.66	14.7
(1,74)	1:508:A:LEU:HD22	2:8:C:LEU:HG	10	14.48	0.66	14.7
(1,74)	1:508:A:LEU:HD23	2:8:C:LEU:HG	10	14.48	0.66	14.7
(3,11)	1:518:A:LEU:CG	2:66:C:THR:H	10	13.83	0.49	13.92
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD11	10	13.66	0.24	13.7
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD12	10	13.66	0.24	13.7
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD13	10	13.66	0.24	13.7
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD21	10	13.66	0.24	13.7
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD22	10	13.66	0.24	13.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD23	10	13.66	0.24	13.7
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG21	10	13.47	0.36	13.55
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG22	10	13.47	0.36	13.55
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG23	10	13.47	0.36	13.55
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG21	10	13.47	0.36	13.55
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG22	10	13.47	0.36	13.55
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG23	10	13.47	0.36	13.55
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG21	10	13.47	0.36	13.55
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG22	10	13.47	0.36	13.55
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG23	10	13.47	0.36	13.55
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD21	10	13.31	0.53	13.4
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD22	10	13.31	0.53	13.4
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD23	10	13.31	0.53	13.4
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD21	10	13.24	0.28	13.1
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD22	10	13.24	0.28	13.1
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD23	10	13.24	0.28	13.1
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD21	10	13.24	0.28	13.1
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD22	10	13.24	0.28	13.1
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD23	10	13.24	0.28	13.1
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD21	10	13.24	0.28	13.1
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD22	10	13.24	0.28	13.1
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD23	10	13.24	0.28	13.1
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD11	10	13.2	0.39	13.38
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD12	10	13.2	0.39	13.38
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD13	10	13.2	0.39	13.38
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD11	10	13.2	0.39	13.38
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD12	10	13.2	0.39	13.38
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD13	10	13.2	0.39	13.38
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD11	10	13.2	0.39	13.38
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD12	10	13.2	0.39	13.38
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD13	10	13.2	0.39	13.38
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD21	10	13.09	0.21	13.18
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD22	10	13.09	0.21	13.18
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD23	10	13.09	0.21	13.18
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD21	10	13.09	0.21	13.18
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD22	10	13.09	0.21	13.18
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD23	10	13.09	0.21	13.18
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD21	10	13.09	0.21	13.18
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD22	10	13.09	0.21	13.18
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD23	10	13.09	0.21	13.18
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD11	10	13.07	0.31	13.08
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD12	10	13.07	0.31	13.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD13	10	13.07	0.31	13.08
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD11	10	13.07	0.31	13.08
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD12	10	13.07	0.31	13.08
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD13	10	13.07	0.31	13.08
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD11	10	13.07	0.31	13.08
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD12	10	13.07	0.31	13.08
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD13	10	13.07	0.31	13.08
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB2	10	13.05	0.59	13.2
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB3	10	13.05	0.59	13.2
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB2	10	13.05	0.59	13.2
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB3	10	13.05	0.59	13.2
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB2	10	13.05	0.59	13.2
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB3	10	13.05	0.59	13.2
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD11	10	13.03	0.29	13.16
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD12	10	13.03	0.29	13.16
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD13	10	13.03	0.29	13.16
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD11	10	13.03	0.29	13.16
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD12	10	13.03	0.29	13.16
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD13	10	13.03	0.29	13.16
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD11	10	13.03	0.29	13.16
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD12	10	13.03	0.29	13.16
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD13	10	13.03	0.29	13.16
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD11	10	12.86	0.56	12.77
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD12	10	12.86	0.56	12.77
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD13	10	12.86	0.56	12.77
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD21	10	12.86	0.75	13.15
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD22	10	12.86	0.75	13.15
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD23	10	12.86	0.75	13.15
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD21	10	12.86	0.75	13.15
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD22	10	12.86	0.75	13.15
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD23	10	12.86	0.75	13.15
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD21	10	12.86	0.75	13.15
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD22	10	12.86	0.75	13.15
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD23	10	12.86	0.75	13.15
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD11	10	12.8	0.46	12.82
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD12	10	12.8	0.46	12.82
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD13	10	12.8	0.46	12.82
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD11	10	12.8	0.46	12.82
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD12	10	12.8	0.46	12.82
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD13	10	12.8	0.46	12.82
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD11	10	12.8	0.46	12.82
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD12	10	12.8	0.46	12.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD13	10	12.8	0.46	12.82
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG21	10	12.72	0.6	12.9
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG22	10	12.72	0.6	12.9
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG23	10	12.72	0.6	12.9
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD21	10	12.63	0.31	12.52
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD22	10	12.63	0.31	12.52
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD23	10	12.63	0.31	12.52
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD21	10	12.63	0.31	12.52
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD22	10	12.63	0.31	12.52
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD23	10	12.63	0.31	12.52
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD21	10	12.63	0.31	12.52
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD22	10	12.63	0.31	12.52
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD23	10	12.63	0.31	12.52
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD11	10	12.6	0.4	12.51
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD12	10	12.6	0.4	12.51
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD13	10	12.6	0.4	12.51
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD11	10	12.6	0.4	12.51
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD12	10	12.6	0.4	12.51
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD13	10	12.6	0.4	12.51
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD11	10	12.6	0.4	12.51
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD12	10	12.6	0.4	12.51
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD13	10	12.6	0.4	12.51
(1,20)	1:544:A:THR:HG21	2:8:B:LEU:HA	10	12.45	0.21	12.49
(1,20)	1:544:A:THR:HG22	2:8:B:LEU:HA	10	12.45	0.21	12.49
(1,20)	1:544:A:THR:HG23	2:8:B:LEU:HA	10	12.45	0.21	12.49
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB2	10	12.16	0.5	12.11
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB3	10	12.16	0.5	12.11
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB2	10	12.16	0.5	12.11
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB3	10	12.16	0.5	12.11
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB2	10	12.16	0.5	12.11
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB3	10	12.16	0.5	12.11
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD21	10	12.14	0.21	12.18
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD22	10	12.14	0.21	12.18
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD23	10	12.14	0.21	12.18
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG21	10	11.79	0.43	11.9
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG22	10	11.79	0.43	11.9
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG23	10	11.79	0.43	11.9
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG21	10	11.79	0.43	11.9
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG22	10	11.79	0.43	11.9
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG23	10	11.79	0.43	11.9
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG21	10	11.79	0.43	11.9
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG22	10	11.79	0.43	11.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG23	10	11.79	0.43	11.9
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD11	10	11.72	0.24	11.75
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD12	10	11.72	0.24	11.75
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD13	10	11.72	0.24	11.75
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	10	11.48	0.5	11.46
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	10	11.48	0.5	11.46
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	10	11.48	0.5	11.46
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	10	11.48	0.5	11.46
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	10	11.48	0.5	11.46
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	10	11.48	0.5	11.46
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG21	10	11.3	0.26	11.46
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG22	10	11.3	0.26	11.46
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG23	10	11.3	0.26	11.46
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG21	10	11.3	0.26	11.46
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG22	10	11.3	0.26	11.46
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG23	10	11.3	0.26	11.46
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG21	10	11.3	0.26	11.46
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG22	10	11.3	0.26	11.46
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG23	10	11.3	0.26	11.46
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD11	10	11.2	0.47	11.26
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD12	10	11.2	0.47	11.26
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD13	10	11.2	0.47	11.26
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD11	10	11.2	0.47	11.26
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD12	10	11.2	0.47	11.26
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD13	10	11.2	0.47	11.26
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD11	10	11.2	0.47	11.26
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD12	10	11.2	0.47	11.26
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD13	10	11.2	0.47	11.26
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD11	10	11.13	0.38	11.3
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD12	10	11.13	0.38	11.3
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD13	10	11.13	0.38	11.3
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD11	10	11.13	0.38	11.3
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD12	10	11.13	0.38	11.3
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD13	10	11.13	0.38	11.3
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD21	10	11.12	0.21	11.12
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD22	10	11.12	0.21	11.12
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD23	10	11.12	0.21	11.12
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG21	10	11.04	0.65	11.12
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG22	10	11.04	0.65	11.12
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG23	10	11.04	0.65	11.12
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG21	10	11.04	0.65	11.12
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG22	10	11.04	0.65	11.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG23	10	11.04	0.65	11.12
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG21	10	11.04	0.65	11.12
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG22	10	11.04	0.65	11.12
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG23	10	11.04	0.65	11.12
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD21	10	10.96	0.41	11.06
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD22	10	10.96	0.41	11.06
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD23	10	10.96	0.41	11.06
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD21	10	10.96	0.41	11.06
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD22	10	10.96	0.41	11.06
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD23	10	10.96	0.41	11.06
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD21	10	10.96	0.41	11.06
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD22	10	10.96	0.41	11.06
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD23	10	10.96	0.41	11.06
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB2	10	10.84	0.28	10.88
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB3	10	10.84	0.28	10.88
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB2	10	10.84	0.28	10.88
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB3	10	10.84	0.28	10.88
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB2	10	10.84	0.28	10.88
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB3	10	10.84	0.28	10.88
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG11	10	10.84	0.39	10.93
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG12	10	10.84	0.39	10.93
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG13	10	10.84	0.39	10.93
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG11	10	10.84	0.39	10.93
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG12	10	10.84	0.39	10.93
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG13	10	10.84	0.39	10.93
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG11	10	10.84	0.39	10.93
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG12	10	10.84	0.39	10.93
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG13	10	10.84	0.39	10.93
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD11	10	10.82	1.02	10.66
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD12	10	10.82	1.02	10.66
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD13	10	10.82	1.02	10.66
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD21	10	10.82	1.02	10.66
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD22	10	10.82	1.02	10.66
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD23	10	10.82	1.02	10.66
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG21	10	10.82	0.23	10.86
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG22	10	10.82	0.23	10.86
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG23	10	10.82	0.23	10.86
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG21	10	10.82	0.23	10.86
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG22	10	10.82	0.23	10.86
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG23	10	10.82	0.23	10.86
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD11	10	10.78	0.2	10.82
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD12	10	10.78	0.2	10.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD13	10	10.78	0.2	10.82
(3,12)	1:518:A:LEU:CG	2:67:C:LEU:H	10	10.58	0.46	10.66
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD21	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD22	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD23	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD21	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD22	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD23	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD21	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD22	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD23	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD21	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD22	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD23	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD21	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD22	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD23	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD21	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD22	10	10.51	0.41	10.54
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD23	10	10.51	0.41	10.54
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD11	10	10.48	0.53	10.43
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD12	10	10.48	0.53	10.43
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD13	10	10.48	0.53	10.43
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD11	10	10.48	0.53	10.43
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD12	10	10.48	0.53	10.43
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD13	10	10.48	0.53	10.43
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD11	10	10.48	0.53	10.43
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD12	10	10.48	0.53	10.43
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD13	10	10.48	0.53	10.43
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD11	10	10.37	0.63	10.43
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD12	10	10.37	0.63	10.43
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD13	10	10.37	0.63	10.43
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD11	10	10.37	0.63	10.43
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD12	10	10.37	0.63	10.43
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD13	10	10.37	0.63	10.43
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD11	10	10.37	0.63	10.43
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD12	10	10.37	0.63	10.43
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD13	10	10.37	0.63	10.43
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD11	10	10.26	0.4	10.34
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD12	10	10.26	0.4	10.34
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD13	10	10.26	0.4	10.34
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD11	10	10.26	0.4	10.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD12	10	10.26	0.4	10.34
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD13	10	10.26	0.4	10.34
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD11	10	10.26	0.4	10.34
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD12	10	10.26	0.4	10.34
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD13	10	10.26	0.4	10.34
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD11	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD12	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD13	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD11	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD12	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD13	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD11	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD12	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD13	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD11	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD12	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD13	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD11	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD12	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD13	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD11	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD12	10	10.25	0.45	10.23
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD13	10	10.25	0.45	10.23
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD21	10	10.22	0.19	10.22
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD22	10	10.22	0.19	10.22
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD23	10	10.22	0.19	10.22
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD21	10	10.22	0.19	10.22
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD22	10	10.22	0.19	10.22
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD23	10	10.22	0.19	10.22
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD21	10	10.22	0.19	10.22
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD22	10	10.22	0.19	10.22
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD23	10	10.22	0.19	10.22
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD11	10	10.05	0.49	10.12
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD12	10	10.05	0.49	10.12
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD13	10	10.05	0.49	10.12
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD21	10	9.98	0.5	10.0
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD22	10	9.98	0.5	10.0
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD23	10	9.98	0.5	10.0
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD21	10	9.98	0.5	10.0
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD22	10	9.98	0.5	10.0
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD23	10	9.98	0.5	10.0
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD21	10	9.83	0.15	9.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD22	10	9.83	0.15	9.82
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD23	10	9.83	0.15	9.82
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD21	10	9.83	0.15	9.82
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD22	10	9.83	0.15	9.82
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD23	10	9.83	0.15	9.82
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD21	10	9.83	0.15	9.82
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD22	10	9.83	0.15	9.82
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD23	10	9.83	0.15	9.82
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD11	10	9.63	0.26	9.62
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD12	10	9.63	0.26	9.62
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD13	10	9.63	0.26	9.62
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD11	10	9.63	0.26	9.62
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD12	10	9.63	0.26	9.62
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD13	10	9.63	0.26	9.62
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD11	10	9.63	0.26	9.62
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD12	10	9.63	0.26	9.62
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD13	10	9.63	0.26	9.62
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD21	10	9.63	0.25	9.61
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD22	10	9.63	0.25	9.61
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD23	10	9.63	0.25	9.61
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG21	10	9.6	0.15	9.63
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG22	10	9.6	0.15	9.63
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG23	10	9.6	0.15	9.63
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG21	10	9.6	0.15	9.63
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG22	10	9.6	0.15	9.63
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG23	10	9.6	0.15	9.63
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG21	10	9.6	0.15	9.63
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG22	10	9.6	0.15	9.63
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG23	10	9.6	0.15	9.63
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD21	10	9.56	0.55	9.7
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD22	10	9.56	0.55	9.7
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD23	10	9.56	0.55	9.7
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD21	10	9.56	0.55	9.7
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD22	10	9.56	0.55	9.7
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD23	10	9.56	0.55	9.7
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD11	10	9.54	1.58	8.95
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD12	10	9.54	1.58	8.95
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD13	10	9.54	1.58	8.95
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD11	10	9.46	0.43	9.36
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD12	10	9.46	0.43	9.36
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD13	10	9.46	0.43	9.36
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD11	10	9.46	0.43	9.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD12	10	9.46	0.43	9.36
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD13	10	9.46	0.43	9.36
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG21	10	9.32	0.37	9.32
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG22	10	9.32	0.37	9.32
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG23	10	9.32	0.37	9.32
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD21	10	9.29	0.22	9.3
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD22	10	9.29	0.22	9.3
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD23	10	9.29	0.22	9.3
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD21	10	9.29	0.22	9.3
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD22	10	9.29	0.22	9.3
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD23	10	9.29	0.22	9.3
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD21	10	9.29	0.22	9.3
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD22	10	9.29	0.22	9.3
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD23	10	9.29	0.22	9.3
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG21	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG22	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG23	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG21	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG22	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG23	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG21	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG22	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG23	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG21	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG22	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG23	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG21	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG22	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG23	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG21	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG22	10	9.26	0.2	9.32
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG23	10	9.26	0.2	9.32
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD21	10	9.22	1.49	8.8
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD22	10	9.22	1.49	8.8
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD23	10	9.22	1.49	8.8
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD11	10	9.14	0.23	9.09
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD12	10	9.14	0.23	9.09
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD13	10	9.14	0.23	9.09
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG21	10	9.11	0.26	9.2
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG22	10	9.11	0.26	9.2
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG23	10	9.11	0.26	9.2
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG21	10	9.05	0.23	9.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG22	10	9.05	0.23	9.1
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG23	10	9.05	0.23	9.1
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG11	10	8.89	0.36	8.93
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG12	10	8.89	0.36	8.93
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG13	10	8.89	0.36	8.93
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD11	10	8.88	0.29	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD12	10	8.88	0.29	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD13	10	8.88	0.29	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD21	10	8.88	0.29	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD22	10	8.88	0.29	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD23	10	8.88	0.29	8.9
(3,1)	1:518:A:LEU:CG	2:6:C:LYS:H	10	8.83	0.48	8.87
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD11	10	8.81	0.18	8.77
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD12	10	8.81	0.18	8.77
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD13	10	8.81	0.18	8.77
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD11	10	8.81	0.18	8.77
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD12	10	8.81	0.18	8.77
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD13	10	8.81	0.18	8.77
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD11	10	8.81	0.18	8.77
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD12	10	8.81	0.18	8.77
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD13	10	8.81	0.18	8.77
(1,64)	1:548:A:ASP:OD2	2:42:B:ARG:NH2	10	8.64	2.0	8.5
(1,64)	1:548:A:ASP:OD1	2:42:B:ARG:NH2	10	8.64	2.0	8.5
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG11	10	8.58	0.23	8.63
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG12	10	8.58	0.23	8.63
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG13	10	8.58	0.23	8.63
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG11	10	8.58	0.23	8.63
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG12	10	8.58	0.23	8.63
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG13	10	8.58	0.23	8.63
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD11	10	8.52	0.69	8.36
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD12	10	8.52	0.69	8.36
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD13	10	8.52	0.69	8.36
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD11	10	8.52	0.69	8.36
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD12	10	8.52	0.69	8.36
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD13	10	8.52	0.69	8.36
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD11	10	8.42	0.71	8.32
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD12	10	8.42	0.71	8.32
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD13	10	8.42	0.71	8.32
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD11	10	8.42	0.71	8.32
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD12	10	8.42	0.71	8.32
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD13	10	8.42	0.71	8.32
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD11	10	8.42	0.71	8.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD12	10	8.42	0.71	8.32
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD13	10	8.42	0.71	8.32
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD11	10	8.4	1.33	7.94
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD12	10	8.4	1.33	7.94
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD13	10	8.4	1.33	7.94
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD11	10	8.4	1.33	7.94
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD12	10	8.4	1.33	7.94
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD13	10	8.4	1.33	7.94
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG11	10	8.26	0.27	8.26
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG12	10	8.26	0.27	8.26
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG13	10	8.26	0.27	8.26
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG11	10	8.26	0.27	8.26
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG12	10	8.26	0.27	8.26
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG13	10	8.26	0.27	8.26
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG11	10	8.26	0.27	8.26
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG12	10	8.26	0.27	8.26
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG13	10	8.26	0.27	8.26
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG21	10	8.2	0.36	8.28
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG22	10	8.2	0.36	8.28
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG23	10	8.2	0.36	8.28
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG21	10	8.2	0.36	8.28
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG22	10	8.2	0.36	8.28
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG23	10	8.2	0.36	8.28
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG11	10	8.14	0.37	8.16
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG12	10	8.14	0.37	8.16
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG13	10	8.14	0.37	8.16
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD21	10	8.14	1.18	8.06
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD22	10	8.14	1.18	8.06
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD23	10	8.14	1.18	8.06
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD21	10	8.14	1.18	8.06
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD22	10	8.14	1.18	8.06
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD23	10	8.14	1.18	8.06
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG21	10	8.06	0.17	8.06
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG22	10	8.06	0.17	8.06
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG23	10	8.06	0.17	8.06
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG21	10	8.06	0.17	8.06
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG22	10	8.06	0.17	8.06
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG23	10	8.06	0.17	8.06
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG21	10	8.06	0.17	8.06
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG22	10	8.06	0.17	8.06
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG23	10	8.06	0.17	8.06
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG21	10	8.0	0.22	8.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG22	10	8.0	0.22	8.04
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG23	10	8.0	0.22	8.04
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD11	10	7.9	0.2	7.86
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD12	10	7.9	0.2	7.86
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD13	10	7.9	0.2	7.86
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD21	10	7.9	0.2	7.86
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD22	10	7.9	0.2	7.86
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD23	10	7.9	0.2	7.86
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD11	10	7.9	0.2	7.86
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD12	10	7.9	0.2	7.86
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD13	10	7.9	0.2	7.86
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD21	10	7.9	0.2	7.86
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD22	10	7.9	0.2	7.86
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD23	10	7.9	0.2	7.86
(1,6)	1:514:A:ALA:HB1	2:73:B:LEU:HG	10	7.78	1.43	7.72
(1,6)	1:514:A:ALA:HB2	2:73:B:LEU:HG	10	7.78	1.43	7.72
(1,6)	1:514:A:ALA:HB3	2:73:B:LEU:HG	10	7.78	1.43	7.72
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD11	10	7.76	0.22	7.77
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD12	10	7.76	0.22	7.77
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD13	10	7.76	0.22	7.77
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD21	10	7.76	0.22	7.77
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD22	10	7.76	0.22	7.77
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD23	10	7.76	0.22	7.77
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD11	10	7.71	0.76	7.83
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD12	10	7.71	0.76	7.83
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD13	10	7.71	0.76	7.83
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD11	10	7.71	0.76	7.83
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD12	10	7.71	0.76	7.83
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD13	10	7.71	0.76	7.83
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD11	10	7.71	0.76	7.83
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD12	10	7.71	0.76	7.83
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD13	10	7.71	0.76	7.83
(1,65)	1:552:A:GLU:OE1	2:42:B:ARG:NH1	10	7.43	2.75	7.1
(1,65)	1:552:A:GLU:OE2	2:42:B:ARG:NH1	10	7.43	2.75	7.1
(3,10)	1:518:A:LEU:CG	2:51:C:GLU:H	10	7.08	0.9	7.1
(3,7)	1:518:A:LEU:CG	2:45:C:PHE:H	10	7.07	0.7	7.04
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD11	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD12	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD13	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD21	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD22	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD23	10	7.05	0.29	7.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD11	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD12	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD13	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD21	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD22	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD23	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD11	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD12	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD13	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD21	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD22	10	7.05	0.29	7.16
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD23	10	7.05	0.29	7.16
(3,13)	1:518:A:LEU:CG	2:68:C:HIS:H	10	7.04	0.6	7.08
(3,2)	1:518:A:LEU:CG	2:7:C:THR:H	10	6.84	0.44	6.88
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG11	10	6.82	0.36	6.92
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG12	10	6.82	0.36	6.92
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG13	10	6.82	0.36	6.92
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG21	10	6.82	0.36	6.92
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG22	10	6.82	0.36	6.92
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG23	10	6.82	0.36	6.92
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG11	10	6.78	0.36	6.78
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG12	10	6.78	0.36	6.78
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG13	10	6.78	0.36	6.78
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG11	10	6.58	0.25	6.69
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG12	10	6.58	0.25	6.69
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG13	10	6.58	0.25	6.69
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB2	10	6.3	0.94	6.43
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB3	10	6.3	0.94	6.43
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB2	10	6.3	0.94	6.43
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB3	10	6.3	0.94	6.43
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB2	10	6.3	0.94	6.43
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB3	10	6.3	0.94	6.43
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG11	10	5.98	0.35	6.04
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG12	10	5.98	0.35	6.04
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG13	10	5.98	0.35	6.04
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG11	10	5.98	0.35	6.04
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG12	10	5.98	0.35	6.04
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG13	10	5.98	0.35	6.04
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD11	10	5.95	1.28	5.76
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD12	10	5.95	1.28	5.76
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD13	10	5.95	1.28	5.76
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD11	10	5.95	1.28	5.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD12	10	5.95	1.28	5.76
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD13	10	5.95	1.28	5.76
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD11	10	5.95	1.28	5.76
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD12	10	5.95	1.28	5.76
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD13	10	5.95	1.28	5.76
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD11	10	5.77	1.87	5.56
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD12	10	5.77	1.87	5.56
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD13	10	5.77	1.87	5.56
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD21	10	5.7	1.19	5.7
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD22	10	5.7	1.19	5.7
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD23	10	5.7	1.19	5.7
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD21	10	5.7	1.19	5.7
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD22	10	5.7	1.19	5.7
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD23	10	5.7	1.19	5.7
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD21	10	5.7	1.19	5.7
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD22	10	5.7	1.19	5.7
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD23	10	5.7	1.19	5.7
(1,3)	1:514:A:ALA:HB1	2:73:B:LEU:HA	10	5.53	0.68	5.48
(1,3)	1:514:A:ALA:HB2	2:73:B:LEU:HA	10	5.53	0.68	5.48
(1,3)	1:514:A:ALA:HB3	2:73:B:LEU:HA	10	5.53	0.68	5.48
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD21	10	5.43	1.57	5.32
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD22	10	5.43	1.57	5.32
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD23	10	5.43	1.57	5.32
(3,9)	1:518:A:LEU:CG	2:50:C:LEU:H	10	5.07	0.79	5.05
(3,6)	1:518:A:LEU:CG	2:44:C:ILE:H	10	4.78	0.54	4.78
(3,14)	1:518:A:LEU:CG	2:69:C:LEU:H	10	4.72	0.56	4.56
(3,8)	1:518:A:LEU:CG	2:49:C:GLN:H	10	4.67	0.96	4.73
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD11	10	3.74	1.19	3.51
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD12	10	3.74	1.19	3.51
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD13	10	3.74	1.19	3.51
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD21	10	3.74	1.19	3.51
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD22	10	3.74	1.19	3.51
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD23	10	3.74	1.19	3.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD11	10	3.74	1.19	3.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD12	10	3.74	1.19	3.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD13	10	3.74	1.19	3.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD21	10	3.74	1.19	3.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD22	10	3.74	1.19	3.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD23	10	3.74	1.19	3.51
(1,101)	1:516:A:THR:HG21	2:73:C:LEU:HA	10	3.3	0.85	3.08
(1,101)	1:516:A:THR:HG22	2:73:C:LEU:HA	10	3.3	0.85	3.08
(1,101)	1:516:A:THR:HG23	2:73:C:LEU:HA	10	3.3	0.85	3.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,5)	1:518:A:LEU:CG	2:43:C:LEU:H	10	2.97	0.66	2.89
(3,4)	1:518:A:LEU:CG	2:9:C:THR:H	10	2.57	0.89	2.59
(3,3)	1:518:A:LEU:CG	2:8:C:LEU:H	10	2.45	0.42	2.5
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD11	10	1.95	0.34	1.96
(1,3018)	2:40:C:GLN:HG3	2:71:C:LEU:HD22	10	1.95	0.34	1.96
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD12	10	1.95	0.34	1.96
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD13	10	1.95	0.34	1.96
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD21	10	1.95	0.34	1.96
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD22	10	1.95	0.34	1.96
(1,254)	1:515:A:SER:HA	1:518:A:LEU:H	10	1.58	0.84	1.8
(1,498)	1:573:A:LEU:H	1:575:A:MET:H	10	1.43	0.24	1.32
(1,1448)	2:1:C:MET:HE1	2:17:C:VAL:HG13	10	1.36	0.09	1.36
(1,1448)	2:1:C:MET:HE2	2:17:C:VAL:HG11	10	1.36	0.09	1.36
(1,1448)	2:1:C:MET:HE2	2:17:C:VAL:HG13	10	1.36	0.09	1.36
(1,1448)	2:1:C:MET:HE3	2:17:C:VAL:HG13	10	1.36	0.09	1.36
(1,1448)	2:1:C:MET:HE3	2:17:C:VAL:HG12	10	1.36	0.09	1.36
(1,1448)	2:1:C:MET:HE1	2:17:C:VAL:HG12	10	1.36	0.09	1.36
(1,1448)	2:1:C:MET:HE2	2:17:C:VAL:HG12	10	1.36	0.09	1.36
(1,1448)	2:1:C:MET:HE3	2:17:C:VAL:HG11	10	1.36	0.09	1.36
(1,3714)	2:1:B:MET:HE1	2:17:B:VAL:HG13	10	1.35	0.12	1.35
(1,3714)	2:1:B:MET:HE3	2:17:B:VAL:HG13	10	1.35	0.12	1.35
(1,3714)	2:1:B:MET:HE1	2:17:B:VAL:HG11	10	1.35	0.12	1.35
(1,3714)	2:1:B:MET:HE3	2:17:B:VAL:HG11	10	1.35	0.12	1.35
(1,3714)	2:1:B:MET:HE1	2:17:B:VAL:HG12	10	1.35	0.12	1.35
(1,3714)	2:1:B:MET:HE2	2:17:B:VAL:HG11	10	1.35	0.12	1.35
(3,15)	1:518:A:LEU:CG	2:70:C:VAL:H	10	1.14	0.57	1.08
(1,3632)	2:66:C:THR:HG23	2:68:C:HIS:HB3	10	1.1	0.15	1.11
(1,3632)	2:70:C:VAL:HG12	2:68:C:HIS:HB3	10	1.1	0.15	1.11
(1,3632)	2:66:C:THR:HG22	2:68:C:HIS:HB3	10	1.1	0.15	1.11
(1,3632)	2:70:C:VAL:HG11	2:68:C:HIS:HB3	10	1.1	0.15	1.11
(1,3632)	2:66:C:THR:HG21	2:68:C:HIS:HB3	10	1.1	0.15	1.11
(1,1447)	2:1:C:MET:HE1	2:17:C:VAL:HG13	10	0.98	0.09	0.98
(1,1447)	2:1:C:MET:HE2	2:17:C:VAL:HG11	10	0.98	0.09	0.98
(1,1447)	2:1:C:MET:HE2	2:17:C:VAL:HG13	10	0.98	0.09	0.98
(1,1447)	2:1:C:MET:HE3	2:17:C:VAL:HG13	10	0.98	0.09	0.98
(1,1447)	2:1:C:MET:HE3	2:17:C:VAL:HG12	10	0.98	0.09	0.98
(1,1447)	2:1:C:MET:HE1	2:17:C:VAL:HG12	10	0.98	0.09	0.98
(1,1447)	2:1:C:MET:HE2	2:17:C:VAL:HG12	10	0.98	0.09	0.98
(1,1447)	2:1:C:MET:HE3	2:17:C:VAL:HG11	10	0.98	0.09	0.98
(1,3713)	2:1:B:MET:HE1	2:17:B:VAL:HG13	10	0.97	0.12	0.96
(1,3713)	2:1:B:MET:HE3	2:17:B:VAL:HG13	10	0.97	0.12	0.96
(1,3713)	2:1:B:MET:HE1	2:17:B:VAL:HG11	10	0.97	0.12	0.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3713)	2:1:B:MET:HE3	2:17:B:VAL:HG11	10	0.97	0.12	0.96
(1,3713)	2:1:B:MET:HE1	2:17:B:VAL:HG12	10	0.97	0.12	0.96
(1,3713)	2:1:B:MET:HE2	2:17:B:VAL:HG11	10	0.97	0.12	0.96
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD11	10	0.89	0.36	0.98
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD22	10	0.89	0.36	0.98
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	10	0.89	0.36	0.98
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD13	10	0.89	0.36	0.98
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD23	10	0.89	0.36	0.98
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD11	10	0.8	0.36	0.9
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD22	10	0.8	0.36	0.9
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	10	0.8	0.36	0.9
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD13	10	0.8	0.36	0.9
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD23	10	0.8	0.36	0.9
(1,1510)	2:1:C:MET:HE3	2:67:C:LEU:HD13	10	0.65	0.29	0.59
(1,1510)	2:1:C:MET:HE1	2:67:C:LEU:HD11	10	0.65	0.29	0.59
(1,1510)	2:1:C:MET:HE1	2:67:C:LEU:HD12	10	0.65	0.29	0.59
(1,1510)	2:1:C:MET:HE3	2:67:C:LEU:HD12	10	0.65	0.29	0.59
(1,1510)	2:1:C:MET:HE2	2:67:C:LEU:HD11	10	0.65	0.29	0.59
(1,1510)	2:1:C:MET:HE2	2:67:C:LEU:HD13	10	0.65	0.29	0.59
(1,1565)	2:3:C:ILE:HD11	2:3:C:ILE:HA	10	0.65	0.05	0.66
(1,1565)	2:3:C:ILE:HD13	2:3:C:ILE:HA	10	0.65	0.05	0.66
(1,1565)	2:3:C:ILE:HD12	2:3:C:ILE:HA	10	0.65	0.05	0.66
(1,3831)	2:3:B:ILE:HD12	2:3:B:ILE:HA	10	0.64	0.03	0.64
(1,3831)	2:3:B:ILE:HD11	2:3:B:ILE:HA	10	0.64	0.03	0.64
(1,3776)	2:1:B:MET:HE3	2:67:B:LEU:HD13	10	0.63	0.24	0.64
(1,3776)	2:1:B:MET:HE2	2:67:B:LEU:HD12	10	0.63	0.24	0.64
(1,3776)	2:1:B:MET:HE3	2:67:B:LEU:HD12	10	0.63	0.24	0.64
(1,3776)	2:1:B:MET:HE2	2:67:B:LEU:HD13	10	0.63	0.24	0.64
(1,3776)	2:1:B:MET:HE1	2:67:B:LEU:HD11	10	0.63	0.24	0.64
(1,3776)	2:1:B:MET:HE3	2:67:B:LEU:HD11	10	0.63	0.24	0.64
(1,3776)	2:1:B:MET:HE1	2:67:B:LEU:HD12	10	0.63	0.24	0.64
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD22	10	0.58	0.22	0.6
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD12	10	0.58	0.22	0.6
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD11	10	0.58	0.22	0.6
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD13	10	0.58	0.22	0.6
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD23	10	0.58	0.22	0.6
(1,1491)	2:1:C:MET:HE1	2:56:C:LEU:HD12	10	0.56	0.16	0.63
(1,1491)	2:1:C:MET:HE2	2:56:C:LEU:HD13	10	0.56	0.16	0.63
(1,1491)	2:1:C:MET:HE3	2:56:C:LEU:HD12	10	0.56	0.16	0.63
(1,1491)	2:1:C:MET:HE2	2:56:C:LEU:HD11	10	0.56	0.16	0.63
(1,1491)	2:1:C:MET:HE3	2:56:C:LEU:HD11	10	0.56	0.16	0.63
(1,3757)	2:1:B:MET:HE1	2:56:B:LEU:HD13	10	0.55	0.22	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3757)	2:1:B:MET:HE3	2:56:B:LEU:HD13	10	0.55	0.22	0.54
(1,3757)	2:1:B:MET:HE1	2:56:B:LEU:HD11	10	0.55	0.22	0.54
(1,3757)	2:1:B:MET:HE3	2:56:B:LEU:HD11	10	0.55	0.22	0.54
(1,3757)	2:1:B:MET:HE2	2:56:B:LEU:HD12	10	0.55	0.22	0.54
(1,3757)	2:1:B:MET:HE3	2:56:B:LEU:HD12	10	0.55	0.22	0.54
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG22	10	0.38	0.11	0.4
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG21	10	0.38	0.11	0.4
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG23	10	0.38	0.11	0.4
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG22	10	0.38	0.11	0.39
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG21	10	0.38	0.11	0.39
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG23	10	0.38	0.11	0.39
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD11	10	0.37	0.05	0.38
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD13	10	0.37	0.05	0.38
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD12	10	0.37	0.05	0.38
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD12	10	0.37	0.03	0.36
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD11	10	0.37	0.03	0.36
(1,1938)	2:14:C:THR:HG23	2:14:C:THR:H	10	0.13	0.02	0.14
(1,1938)	2:14:C:THR:HG21	2:14:C:THR:H	10	0.13	0.02	0.14
(1,1938)	2:14:C:THR:HG22	2:14:C:THR:H	10	0.13	0.02	0.14
(2,4)	1:484:A:LYS:O	1:488:A:ALA:N	9	0.92	0.43	1.1
(2,3)	1:484:A:LYS:O	1:488:A:ALA:H	9	0.85	0.45	1.02
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD12	9	0.76	0.36	0.68
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD21	9	0.76	0.36	0.68
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD22	9	0.76	0.36	0.68
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	9	0.76	0.36	0.68
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD11	9	0.75	0.31	0.68
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	9	0.75	0.31	0.68
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD12	9	0.75	0.31	0.68
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD21	9	0.75	0.31	0.68
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	9	0.75	0.31	0.68
(1,5309)	2:41:B:GLN:H	2:71:B:LEU:HD11	9	0.65	0.16	0.62
(1,5309)	2:41:B:GLN:H	2:69:B:LEU:HD12	9	0.65	0.16	0.62
(1,5309)	2:41:B:GLN:H	2:71:B:LEU:HD13	9	0.65	0.16	0.62
(1,5309)	2:41:B:GLN:H	2:71:B:LEU:HD22	9	0.65	0.16	0.62
(1,5309)	2:41:B:GLN:H	2:69:B:LEU:HD13	9	0.65	0.16	0.62
(1,5309)	2:41:B:GLN:H	2:69:B:LEU:HD11	9	0.65	0.16	0.62
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG13	9	0.58	0.11	0.6
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG11	9	0.58	0.11	0.6
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG12	9	0.58	0.11	0.6
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD22	9	0.56	0.17	0.51
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD21	9	0.56	0.17	0.51
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD23	9	0.56	0.17	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD11	9	0.56	0.17	0.51
(1,1490)	2:1:C:MET:HE2	2:56:C:LEU:HD13	9	0.42	0.12	0.46
(1,1490)	2:1:C:MET:HE3	2:56:C:LEU:HD12	9	0.42	0.12	0.46
(1,1490)	2:1:C:MET:HE2	2:56:C:LEU:HD11	9	0.42	0.12	0.46
(1,1490)	2:1:C:MET:HE3	2:56:C:LEU:HD11	9	0.42	0.12	0.46
(1,1490)	2:1:C:MET:HE1	2:56:C:LEU:HD12	9	0.42	0.12	0.46
(1,1533)	2:68:C:HIS:HA	2:5:C:VAL:HG12	9	0.38	0.13	0.32
(1,1533)	2:68:C:HIS:HA	2:5:C:VAL:HG13	9	0.38	0.13	0.32
(1,1533)	2:2:C:GLN:HA	2:17:C:VAL:HG13	9	0.38	0.13	0.32
(1,1533)	2:68:C:HIS:HA	2:5:C:VAL:HG11	9	0.38	0.13	0.32
(1,3697)	2:1:B:MET:HE3	2:3:B:ILE:HD12	9	0.3	0.09	0.32
(1,3697)	2:1:B:MET:HE3	2:3:B:ILE:HD11	9	0.3	0.09	0.32
(1,3697)	2:1:B:MET:HE2	2:3:B:ILE:HD11	9	0.3	0.09	0.32
(1,3697)	2:1:B:MET:HE1	2:3:B:ILE:HD11	9	0.3	0.09	0.32
(1,3716)	2:1:B:MET:HE3	2:17:B:VAL:HG21	9	0.18	0.06	0.17
(1,3716)	2:1:B:MET:HE1	2:17:B:VAL:HG23	9	0.18	0.06	0.17
(1,3716)	2:1:B:MET:HE3	2:17:B:VAL:HG22	9	0.18	0.06	0.17
(1,3716)	2:1:B:MET:HE1	2:17:B:VAL:HG22	9	0.18	0.06	0.17
(1,3716)	2:1:B:MET:HE1	2:17:B:VAL:HG21	9	0.18	0.06	0.17
(1,3716)	2:1:B:MET:HE2	2:17:B:VAL:HG21	9	0.18	0.06	0.17
(1,4204)	2:14:B:THR:HG21	2:14:B:THR:H	9	0.16	0.03	0.15
(1,4204)	2:14:B:THR:HG23	2:14:B:THR:H	9	0.16	0.03	0.15
(1,4204)	2:14:B:THR:HG22	2:14:B:THR:H	9	0.16	0.03	0.15
(1,4105)	2:6:B:LYS:HG3	2:66:B:THR:HG21	8	0.93	0.16	1.0
(1,4105)	2:6:B:LYS:HG3	2:66:B:THR:HG23	8	0.93	0.16	1.0
(1,1839)	2:6:C:LYS:HG3	2:66:C:THR:HG21	8	0.83	0.26	0.86
(1,1839)	2:6:C:LYS:HG3	2:66:C:THR:HG23	8	0.83	0.26	0.86
(1,1839)	2:6:C:LYS:HG3	2:66:C:THR:HG22	8	0.83	0.26	0.86
(1,1839)	2:6:C:LYS:HG2	2:66:C:THR:HG23	8	0.83	0.26	0.86
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD12	8	0.75	0.3	0.66
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD21	8	0.75	0.3	0.66
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD22	8	0.75	0.3	0.66
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	8	0.75	0.3	0.66
(1,4103)	2:6:B:LYS:HG3	2:66:B:THR:HG21	8	0.62	0.16	0.7
(1,4103)	2:6:B:LYS:HG3	2:66:B:THR:HG23	8	0.62	0.16	0.7
(1,1837)	2:6:C:LYS:HG3	2:66:C:THR:HG21	8	0.52	0.26	0.54
(1,1837)	2:6:C:LYS:HG3	2:66:C:THR:HG23	8	0.52	0.26	0.54
(1,1837)	2:6:C:LYS:HG3	2:66:C:THR:HG22	8	0.52	0.26	0.54
(1,1837)	2:6:C:LYS:HG2	2:66:C:THR:HG23	8	0.52	0.26	0.54
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD11	8	0.51	0.27	0.4
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	8	0.51	0.27	0.4
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD12	8	0.51	0.27	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD21	8	0.51	0.27	0.4
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	8	0.51	0.27	0.4
(1,4104)	2:6:B:LYS:HG3	2:66:B:THR:HG21	8	0.51	0.16	0.58
(1,4104)	2:6:B:LYS:HG3	2:66:B:THR:HG23	8	0.51	0.16	0.58
(1,3756)	2:1:B:MET:HE3	2:56:B:LEU:HD13	8	0.46	0.17	0.48
(1,3756)	2:1:B:MET:HE1	2:56:B:LEU:HD11	8	0.46	0.17	0.48
(1,3756)	2:1:B:MET:HE3	2:56:B:LEU:HD11	8	0.46	0.17	0.48
(1,3756)	2:1:B:MET:HE1	2:56:B:LEU:HD13	8	0.46	0.17	0.48
(1,3756)	2:1:B:MET:HE2	2:56:B:LEU:HD12	8	0.46	0.17	0.48
(1,3756)	2:1:B:MET:HE3	2:56:B:LEU:HD12	8	0.46	0.17	0.48
(1,120)	1:503:A:ASP:H	1:506:A:LEU:H	8	0.45	0.24	0.44
(1,5300)	2:41:B:GLN:HA	2:71:B:LEU:HD11	8	0.33	0.17	0.36
(1,5300)	2:41:B:GLN:HA	2:69:B:LEU:HD12	8	0.33	0.17	0.36
(1,5300)	2:41:B:GLN:HA	2:71:B:LEU:HD21	8	0.33	0.17	0.36
(1,5300)	2:41:B:GLN:HA	2:69:B:LEU:HD13	8	0.33	0.17	0.36
(1,5300)	2:41:B:GLN:HA	2:69:B:LEU:HD11	8	0.33	0.17	0.36
(1,5300)	2:41:B:GLN:HA	2:71:B:LEU:HD13	8	0.33	0.17	0.36
(1,1450)	2:1:C:MET:HE2	2:17:C:VAL:HG21	8	0.18	0.05	0.17
(1,1450)	2:1:C:MET:HE3	2:17:C:VAL:HG21	8	0.18	0.05	0.17
(1,1450)	2:1:C:MET:HE3	2:17:C:VAL:HG23	8	0.18	0.05	0.17
(1,1450)	2:1:C:MET:HE1	2:17:C:VAL:HG22	8	0.18	0.05	0.17
(1,5284)	2:40:B:GLN:HG3	2:71:B:LEU:HD12	7	0.89	0.26	1.0
(1,5284)	2:40:B:GLN:HG3	2:71:B:LEU:HD21	7	0.89	0.26	1.0
(1,5284)	2:40:B:GLN:HG3	2:71:B:LEU:HD23	7	0.89	0.26	1.0
(1,5284)	2:40:B:GLN:HG3	2:71:B:LEU:HD22	7	0.89	0.26	1.0
(1,5183)	2:36:B:ILE:HG23	2:71:B:LEU:HD13	7	0.61	0.21	0.54
(1,5183)	2:36:B:ILE:HG22	2:71:B:LEU:HD11	7	0.61	0.21	0.54
(1,5183)	2:36:B:ILE:HG22	2:71:B:LEU:HD23	7	0.61	0.21	0.54
(1,5183)	2:36:B:ILE:HG23	2:71:B:LEU:HD23	7	0.61	0.21	0.54
(1,5183)	2:36:B:ILE:HG21	2:71:B:LEU:HD12	7	0.61	0.21	0.54
(1,4014)	2:5:B:VAL:HG23	2:15:B:LEU:HG	7	0.53	0.22	0.52
(1,4014)	2:5:B:VAL:HG22	2:15:B:LEU:HG	7	0.53	0.22	0.52
(1,4014)	2:5:B:VAL:HG23	2:13:B:ILE:HG13	7	0.53	0.22	0.52
(1,4014)	2:5:B:VAL:HG21	2:13:B:ILE:HG13	7	0.53	0.22	0.52
(1,4014)	2:5:B:VAL:HG22	2:13:B:ILE:HG13	7	0.53	0.22	0.52
(1,412)	1:547:A:MET:HE1	1:548:A:ASP:H	7	0.48	0.16	0.53
(1,412)	1:547:A:MET:HE2	1:548:A:ASP:H	7	0.48	0.16	0.53
(1,412)	1:547:A:MET:HE3	1:548:A:ASP:H	7	0.48	0.16	0.53
(1,4031)	2:17:B:VAL:HG12	2:29:B:LYS:HG3	7	0.43	0.16	0.36
(1,4031)	2:17:B:VAL:HG11	2:29:B:LYS:HG3	7	0.43	0.16	0.36
(1,4031)	2:17:B:VAL:HG12	2:29:B:LYS:HG2	7	0.43	0.16	0.36
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD13	7	0.4	0.15	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD12	7	0.4	0.15	0.44
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD22	7	0.4	0.15	0.44
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD21	7	0.4	0.15	0.44
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD23	7	0.4	0.15	0.44
(1,1620)	2:29:C:LYS:HA	2:33:C:LYS:HE2	7	0.34	0.14	0.3
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD22	7	0.27	0.13	0.27
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD12	7	0.27	0.13	0.27
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD13	7	0.27	0.13	0.27
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD11	7	0.27	0.13	0.27
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD23	7	0.27	0.13	0.27
(1,3712)	2:1:B:MET:HE3	2:17:B:VAL:HB	7	0.18	0.06	0.18
(1,3712)	2:1:B:MET:HE1	2:17:B:VAL:HB	7	0.18	0.06	0.18
(1,3712)	2:1:B:MET:HE2	2:17:B:VAL:HB	7	0.18	0.06	0.18
(1,1388)	1:599:A:ILE:HD12	1:562:A:TRP:HZ3	6	1.16	0.6	1.16
(1,1388)	1:599:A:ILE:HD11	1:562:A:TRP:HH2	6	1.16	0.6	1.16
(1,1388)	1:599:A:ILE:HD11	1:562:A:TRP:HZ3	6	1.16	0.6	1.16
(1,1388)	1:599:A:ILE:HD13	1:562:A:TRP:HZ3	6	1.16	0.6	1.16
(3,259)	2:66:B:THR:HG23	2:67:B:LEU:HD22	6	0.82	0.05	0.8
(3,259)	2:66:B:THR:HG21	2:67:B:LEU:HD21	6	0.82	0.05	0.8
(3,259)	2:66:B:THR:HG23	2:67:B:LEU:HD21	6	0.82	0.05	0.8
(3,259)	2:66:B:THR:HG22	2:67:B:LEU:HD21	6	0.82	0.05	0.8
(1,863)	1:520:A:ILE:HG12	1:562:A:TRP:HE3	6	0.72	0.23	0.68
(1,863)	1:520:A:ILE:HG13	1:562:A:TRP:HD1	6	0.72	0.23	0.68
(1,863)	1:520:A:ILE:HG13	1:562:A:TRP:HE3	6	0.72	0.23	0.68
(1,1838)	2:6:C:LYS:HG3	2:66:C:THR:HG21	6	0.52	0.18	0.54
(1,1838)	2:6:C:LYS:HG3	2:66:C:THR:HG23	6	0.52	0.18	0.54
(1,1838)	2:6:C:LYS:HG3	2:66:C:THR:HG22	6	0.52	0.18	0.54
(1,1838)	2:6:C:LYS:HG2	2:66:C:THR:HG23	6	0.52	0.18	0.54
(3,209)	2:27:B:LYS:HE2	2:69:B:LEU:HD11	6	0.46	0.4	0.34
(3,209)	2:27:B:LYS:HE2	2:69:B:LEU:HD12	6	0.46	0.4	0.34
(1,3015)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	6	0.42	0.25	0.42
(1,3015)	2:40:C:GLN:HB3	2:71:C:LEU:HD12	6	0.42	0.25	0.42
(1,3015)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	6	0.42	0.25	0.42
(1,2842)	2:34:C:GLU:HG3	2:69:C:LEU:HD12	6	0.4	0.2	0.44
(1,2842)	2:34:C:GLU:HG3	2:69:C:LEU:HD23	6	0.4	0.2	0.44
(1,2842)	2:34:C:GLU:HG3	2:69:C:LEU:HD21	6	0.4	0.2	0.44
(1,2842)	2:34:C:GLU:HG3	2:69:C:LEU:HD13	6	0.4	0.2	0.44
(1,2054)	2:15:C:LEU:HD22	2:29:C:LYS:HG2	6	0.38	0.12	0.4
(1,2054)	2:15:C:LEU:HD23	2:29:C:LYS:HG2	6	0.38	0.12	0.4
(1,2054)	2:15:C:LEU:HD21	2:29:C:LYS:HG2	6	0.38	0.12	0.4
(1,5299)	2:41:B:GLN:HA	2:71:B:LEU:HD11	6	0.36	0.13	0.38
(1,5299)	2:41:B:GLN:HA	2:69:B:LEU:HD12	6	0.36	0.13	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5299)	2:41:B:GLN:HA	2:71:B:LEU:HD21	6	0.36	0.13	0.38
(1,5299)	2:41:B:GLN:HA	2:69:B:LEU:HD13	6	0.36	0.13	0.38
(1,3017)	2:40:C:GLN:HB2	2:71:C:LEU:HD11	6	0.3	0.26	0.2
(1,3017)	2:40:C:GLN:HB2	2:71:C:LEU:HD22	6	0.3	0.26	0.2
(1,3017)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	6	0.3	0.26	0.2
(1,3017)	2:40:C:GLN:HB2	2:71:C:LEU:HD23	6	0.3	0.26	0.2
(3,26)	2:2:C:GLN:HG2	2:3:C:ILE:HA	6	0.27	0.04	0.28
(3,26)	2:2:C:GLN:HG3	2:3:C:ILE:HA	6	0.27	0.04	0.28
(1,4102)	2:6:B:LYS:HG3	2:66:B:THR:HG21	6	0.27	0.03	0.26
(1,4102)	2:6:B:LYS:HG3	2:66:B:THR:HG23	6	0.27	0.03	0.26
(1,2050)	2:15:C:LEU:HD22	2:29:C:LYS:HA	6	0.26	0.14	0.24
(1,2050)	2:15:C:LEU:HD21	2:29:C:LYS:HA	6	0.26	0.14	0.24
(1,2050)	2:15:C:LEU:HD23	2:29:C:LYS:HA	6	0.26	0.14	0.24
(1,2050)	2:15:C:LEU:HD11	2:29:C:LYS:HA	6	0.26	0.14	0.24
(1,3738)	2:28:B:ALA:HB3	2:25:B:ASN:HA	6	0.18	0.03	0.18
(1,3738)	2:28:B:ALA:HB1	2:25:B:ASN:HA	6	0.18	0.03	0.18
(1,3738)	2:28:B:ALA:HB2	2:25:B:ASN:HA	6	0.18	0.03	0.18
(1,261)	1:516:A:THR:HA	1:518:A:LEU:H	5	0.75	0.19	0.67
(1,2917)	2:36:C:ILE:HG21	2:71:C:LEU:HD11	5	0.58	0.17	0.65
(1,2917)	2:36:C:ILE:HG21	2:71:C:LEU:HD22	5	0.58	0.17	0.65
(1,2917)	2:36:C:ILE:HG23	2:71:C:LEU:HD21	5	0.58	0.17	0.65
(1,2917)	2:36:C:ILE:HG21	2:71:C:LEU:HD23	5	0.58	0.17	0.65
(1,2917)	2:36:C:ILE:HG21	2:71:C:LEU:HD21	5	0.58	0.17	0.65
(1,505)	1:575:A:MET:HE1	1:575:A:MET:H	5	0.5	0.12	0.56
(1,505)	1:575:A:MET:HE2	1:575:A:MET:H	5	0.5	0.12	0.56
(1,505)	1:575:A:MET:HE3	1:575:A:MET:H	5	0.5	0.12	0.56
(1,4012)	2:5:B:VAL:HG23	2:15:B:LEU:HG	5	0.49	0.16	0.55
(1,4012)	2:5:B:VAL:HG23	2:13:B:ILE:HG13	5	0.49	0.16	0.55
(1,4012)	2:5:B:VAL:HG21	2:13:B:ILE:HG13	5	0.49	0.16	0.55
(1,4012)	2:5:B:VAL:HG22	2:13:B:ILE:HG13	5	0.49	0.16	0.55
(1,1431)	2:1:C:MET:HE1	2:3:C:ILE:HD13	5	0.31	0.09	0.33
(1,1431)	2:1:C:MET:HE2	2:3:C:ILE:HD11	5	0.31	0.09	0.33
(1,1431)	2:1:C:MET:HE1	2:3:C:ILE:HD12	5	0.31	0.09	0.33
(1,253)	1:515:A:SER:HA	1:517:A:ASP:H	5	0.3	0.2	0.27
(1,4337)	2:15:B:LEU:HD23	2:33:B:LYS:HD2	5	0.3	0.17	0.26
(1,4337)	2:15:B:LEU:HD11	2:33:B:LYS:HD2	5	0.3	0.17	0.26
(1,4337)	2:15:B:LEU:HD13	2:33:B:LYS:HD2	5	0.3	0.17	0.26
(1,4337)	2:15:B:LEU:HD21	2:33:B:LYS:HD2	5	0.3	0.17	0.26
(1,3033)	2:41:C:GLN:HA	2:69:C:LEU:HD12	5	0.29	0.11	0.25
(1,3033)	2:41:C:GLN:HA	2:69:C:LEU:HD13	5	0.29	0.11	0.25
(1,3033)	2:41:C:GLN:HA	2:69:C:LEU:HD11	5	0.29	0.11	0.25
(1,3033)	2:41:C:GLN:HA	2:69:C:LEU:HD23	5	0.29	0.11	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1765)	2:17:C:VAL:HG12	2:29:C:LYS:HG3	5	0.25	0.14	0.22
(1,1765)	2:17:C:VAL:HG11	2:29:C:LYS:HG3	5	0.25	0.14	0.22
(1,1765)	2:17:C:VAL:HG13	2:29:C:LYS:HG3	5	0.25	0.14	0.22
(1,1747)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	5	0.25	0.07	0.3
(1,1747)	2:5:C:VAL:HG22	2:13:C:ILE:HG13	5	0.25	0.07	0.3
(1,1446)	2:1:C:MET:HE2	2:17:C:VAL:HB	5	0.2	0.06	0.2
(1,1446)	2:1:C:MET:HE3	2:17:C:VAL:HB	5	0.2	0.06	0.2
(1,1446)	2:1:C:MET:HE1	2:17:C:VAL:HB	5	0.2	0.06	0.2
(3,139)	2:66:C:THR:HG23	2:67:C:LEU:HD23	4	0.62	0.15	0.64
(3,139)	2:66:C:THR:HG22	2:67:C:LEU:HD21	4	0.62	0.15	0.64
(3,139)	2:66:C:THR:HG21	2:67:C:LEU:HD22	4	0.62	0.15	0.64
(3,139)	2:66:C:THR:HG22	2:67:C:LEU:HD12	4	0.62	0.15	0.64
(3,89)	2:27:C:LYS:HE2	2:69:C:LEU:HD11	4	0.57	0.27	0.48
(3,89)	2:27:C:LYS:HE2	2:69:C:LEU:HD12	4	0.57	0.27	0.48
(1,2843)	2:34:C:GLU:HG3	2:69:C:LEU:HD12	4	0.44	0.09	0.46
(1,2843)	2:34:C:GLU:HG3	2:69:C:LEU:HD21	4	0.44	0.09	0.46
(1,2843)	2:34:C:GLU:HG3	2:69:C:LEU:HD23	4	0.44	0.09	0.46
(1,2843)	2:34:C:GLU:HG3	2:69:C:LEU:HD13	4	0.44	0.09	0.46
(3,153)	2:3:B:ILE:HG22	2:67:B:LEU:HG	4	0.43	0.15	0.41
(3,153)	2:3:B:ILE:HG23	2:67:B:LEU:HG	4	0.43	0.15	0.41
(3,33)	2:3:C:ILE:HG23	2:67:C:LEU:HG	4	0.36	0.21	0.35
(3,33)	2:3:C:ILE:HG21	2:67:C:LEU:HG	4	0.36	0.21	0.35
(3,33)	2:3:C:ILE:HG22	2:67:C:LEU:HG	4	0.36	0.21	0.35
(1,2071)	2:15:C:LEU:HD23	2:33:C:LYS:HD2	4	0.35	0.04	0.36
(1,2071)	2:15:C:LEU:HD21	2:33:C:LYS:HD2	4	0.35	0.04	0.36
(1,5898)	2:70:B:VAL:HG12	2:68:B:HIS:HB3	4	0.34	0.2	0.34
(1,5898)	2:70:B:VAL:HG11	2:68:B:HIS:HB3	4	0.34	0.2	0.34
(1,1772)	2:5:C:VAL:HA	2:66:C:THR:HG23	4	0.32	0.09	0.34
(1,1772)	2:5:C:VAL:HA	2:66:C:THR:HG21	4	0.32	0.09	0.34
(1,1772)	2:5:C:VAL:HA	2:66:C:THR:HG22	4	0.32	0.09	0.34
(1,3800)	2:2:B:GLN:HE22	2:14:B:THR:HG21	4	0.32	0.22	0.27
(1,3800)	2:2:B:GLN:HE22	2:14:B:THR:HG23	4	0.32	0.22	0.27
(1,1773)	2:5:C:VAL:HA	2:66:C:THR:HG23	4	0.32	0.09	0.33
(1,1773)	2:5:C:VAL:HA	2:66:C:THR:HG21	4	0.32	0.09	0.33
(1,1773)	2:5:C:VAL:HA	2:66:C:THR:HG22	4	0.32	0.09	0.33
(1,1836)	2:6:C:LYS:HG2	2:66:C:THR:HG23	4	0.31	0.1	0.32
(1,1836)	2:6:C:LYS:HG3	2:66:C:THR:HG21	4	0.31	0.1	0.32
(1,1836)	2:6:C:LYS:HG3	2:66:C:THR:HG23	4	0.31	0.1	0.32
(1,5184)	2:36:B:ILE:HG22	2:71:B:LEU:HD23	4	0.31	0.2	0.24
(1,5184)	2:36:B:ILE:HG22	2:71:B:LEU:HD11	4	0.31	0.2	0.24
(1,5184)	2:36:B:ILE:HG21	2:71:B:LEU:HD12	4	0.31	0.2	0.24
(1,4100)	2:6:B:LYS:HD2	2:66:B:THR:HG21	4	0.25	0.14	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4100)	2:6:B:LYS:HD2	2:66:B:THR:HG22	4	0.25	0.14	0.22
(1,2918)	2:36:C:ILE:HG21	2:71:C:LEU:HD11	4	0.25	0.04	0.25
(1,2918)	2:36:C:ILE:HG21	2:71:C:LEU:HD21	4	0.25	0.04	0.25
(1,2918)	2:36:C:ILE:HG23	2:71:C:LEU:HD21	4	0.25	0.04	0.25
(1,2918)	2:36:C:ILE:HG21	2:71:C:LEU:HD23	4	0.25	0.04	0.25
(1,1881)	2:7:C:THR:HA	2:69:C:LEU:HD23	4	0.23	0.07	0.22
(1,1881)	2:7:C:THR:HA	2:69:C:LEU:HD21	4	0.23	0.07	0.22
(1,3886)	2:29:B:LYS:HA	2:33:B:LYS:HE2	4	0.22	0.08	0.22
(1,3886)	2:29:B:LYS:HA	2:33:B:LYS:HE3	4	0.22	0.08	0.22
(3,146)	2:2:B:GLN:HG2	2:3:B:ILE:HA	4	0.21	0.06	0.2
(1,3798)	2:68:B:HIS:HA	2:5:B:VAL:HG13	4	0.18	0.06	0.17
(1,3798)	2:68:B:HIS:HA	2:5:B:VAL:HG11	4	0.18	0.06	0.17
(1,3798)	2:68:B:HIS:HA	2:5:B:VAL:HG12	4	0.18	0.06	0.17
(1,4320)	2:15:B:LEU:HD23	2:29:B:LYS:HG2	4	0.18	0.09	0.14
(1,4320)	2:15:B:LEU:HD13	2:29:B:LYS:HG3	4	0.18	0.09	0.14
(1,4320)	2:15:B:LEU:HD22	2:29:B:LYS:HG2	4	0.18	0.09	0.14
(1,5360)	2:43:B:LEU:HD21	2:67:B:LEU:HB3	3	0.69	0.11	0.66
(1,5360)	2:43:B:LEU:HD22	2:67:B:LEU:HB3	3	0.69	0.11	0.66
(1,5108)	2:34:B:GLU:HG3	2:69:B:LEU:HD21	3	0.67	0.08	0.66
(1,5108)	2:34:B:GLU:HG3	2:69:B:LEU:HD23	3	0.67	0.08	0.66
(1,5109)	2:34:B:GLU:HG3	2:69:B:LEU:HD21	3	0.57	0.08	0.56
(1,5109)	2:34:B:GLU:HG3	2:69:B:LEU:HD23	3	0.57	0.08	0.56
(1,3048)	2:42:C:ARG:HA	2:69:C:LEU:HD22	3	0.49	0.07	0.46
(1,3048)	2:42:C:ARG:HA	2:69:C:LEU:HD23	3	0.49	0.07	0.46
(1,1835)	2:6:C:LYS:HE3	2:66:C:THR:HG23	3	0.48	0.19	0.36
(1,1835)	2:6:C:LYS:HE3	2:66:C:THR:HG21	3	0.48	0.19	0.36
(1,5107)	2:34:B:GLU:HG3	2:36:B:ILE:HG13	3	0.44	0.06	0.4
(1,5107)	2:34:B:GLU:HG2	2:36:B:ILE:HG13	3	0.44	0.06	0.4
(1,3014)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	3	0.38	0.06	0.39
(1,3014)	2:40:C:GLN:HB3	2:71:C:LEU:HD12	3	0.38	0.06	0.39
(1,5283)	2:40:B:GLN:HB2	2:71:B:LEU:HD22	3	0.37	0.17	0.32
(1,5283)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	3	0.37	0.17	0.32
(1,1834)	2:6:C:LYS:HD2	2:66:C:THR:HG21	3	0.3	0.11	0.37
(1,1834)	2:6:C:LYS:HD2	2:66:C:THR:HG23	3	0.3	0.11	0.37
(3,24)	2:1:C:MET:HE2	2:67:C:LEU:HD11	3	0.3	0.22	0.17
(3,24)	2:1:C:MET:HE1	2:67:C:LEU:HD12	3	0.3	0.22	0.17
(3,24)	2:1:C:MET:HE3	2:67:C:LEU:HD12	3	0.3	0.22	0.17
(1,4030)	2:17:B:VAL:HG11	2:29:B:LYS:HG3	3	0.26	0.14	0.2
(1,4030)	2:17:B:VAL:HG12	2:29:B:LYS:HG2	3	0.26	0.14	0.2
(1,4260)	2:13:B:ILE:HG12	2:34:B:GLU:HG3	3	0.21	0.05	0.2
(1,4205)	2:14:B:THR:HG22	2:15:B:LEU:H	3	0.19	0.07	0.18
(1,4205)	2:14:B:THR:HG23	2:15:B:LEU:H	3	0.19	0.07	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1509)	2:1:C:MET:HG3	2:63:C:LYS:HA	3	0.16	0.02	0.17
(1,1557)	2:68:C:HIS:HA	2:66:C:THR:HG22	3	0.16	0.05	0.15
(1,1557)	2:68:C:HIS:HA	2:66:C:THR:HG23	3	0.16	0.05	0.15
(1,5908)	2:67:B:LEU:HB3	2:68:B:HIS:H	3	0.16	0.03	0.17
(1,1749)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	3	0.16	0.0	0.16
(1,1749)	2:5:C:VAL:HG22	2:13:C:ILE:HG13	3	0.16	0.0	0.16
(1,3642)	2:67:C:LEU:HB3	2:68:C:HIS:H	3	0.15	0.03	0.15
(1,1472)	2:28:C:ALA:HB2	2:25:C:ASN:HA	3	0.15	0.05	0.14
(1,1472)	2:28:C:ALA:HB3	2:25:C:ASN:HA	3	0.15	0.05	0.14
(1,1472)	2:28:C:ALA:HB1	2:25:C:ASN:HA	3	0.15	0.05	0.14
(1,3775)	2:1:B:MET:HG3	2:63:B:LYS:HA	3	0.14	0.03	0.12
(1,1887)	2:7:C:THR:HB	2:69:C:LEU:HD23	3	0.13	0.01	0.12
(1,1887)	2:7:C:THR:HB	2:71:C:LEU:HD13	3	0.13	0.01	0.12
(1,1887)	2:7:C:THR:HB	2:69:C:LEU:HD21	3	0.13	0.01	0.12
(1,2247)	2:52:C:ASP:HB2	2:24:C:GLU:HB2	3	0.11	0.0	0.11
(1,4745)	2:40:B:GLN:HG2	2:39:B:ASP:H	2	0.8	0.2	0.8
(1,248)	1:515:A:SER:H	1:517:A:ASP:H	2	0.73	0.04	0.73
(1,100)	1:516:A:THR:HG21	2:72:C:ARG:HD2	2	0.7	0.5	0.7
(1,100)	1:516:A:THR:HG21	2:72:C:ARG:HD3	2	0.7	0.5	0.7
(1,100)	1:516:A:THR:HG22	2:72:C:ARG:HD2	2	0.7	0.5	0.7
(1,100)	1:516:A:THR:HG22	2:72:C:ARG:HD3	2	0.7	0.5	0.7
(1,100)	1:516:A:THR:HG23	2:72:C:ARG:HD2	2	0.7	0.5	0.7
(1,100)	1:516:A:THR:HG23	2:72:C:ARG:HD3	2	0.7	0.5	0.7
(1,3094)	2:43:C:LEU:HD21	2:67:C:LEU:HB3	2	0.68	0.08	0.68
(1,1748)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	2	0.65	0.1	0.65
(1,1748)	2:5:C:VAL:HG21	2:15:C:LEU:HG	2	0.65	0.1	0.65
(1,1746)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	2	0.49	0.1	0.49
(1,1746)	2:5:C:VAL:HG21	2:15:C:LEU:HG	2	0.49	0.1	0.49
(3,34)	2:3:C:ILE:HG13	2:67:C:LEU:HB2	2	0.42	0.08	0.42
(1,99)	1:516:A:THR:HG21	2:72:C:ARG:HG2	2	0.42	0.06	0.42
(1,99)	1:516:A:THR:HG21	2:72:C:ARG:HG3	2	0.42	0.06	0.42
(1,99)	1:516:A:THR:HG22	2:72:C:ARG:HG2	2	0.42	0.06	0.42
(1,99)	1:516:A:THR:HG22	2:72:C:ARG:HG3	2	0.42	0.06	0.42
(1,99)	1:516:A:THR:HG23	2:72:C:ARG:HG2	2	0.42	0.06	0.42
(1,99)	1:516:A:THR:HG23	2:72:C:ARG:HG3	2	0.42	0.06	0.42
(1,5314)	2:42:B:ARG:HA	2:69:B:LEU:HD11	2	0.41	0.02	0.41
(1,5314)	2:42:B:ARG:HA	2:69:B:LEU:HD21	2	0.41	0.02	0.41
(1,4230)	2:13:B:ILE:HG23	2:15:B:LEU:HD12	2	0.4	0.17	0.4
(1,4230)	2:13:B:ILE:HG22	2:15:B:LEU:HD22	2	0.4	0.17	0.4
(1,1534)	2:2:C:GLN:HE22	2:14:C:THR:HG21	2	0.34	0.06	0.34
(1,1534)	2:2:C:GLN:HE22	2:14:C:THR:HG22	2	0.34	0.06	0.34
(3,144)	2:1:B:MET:HE3	2:67:B:LEU:HD13	2	0.26	0.16	0.26

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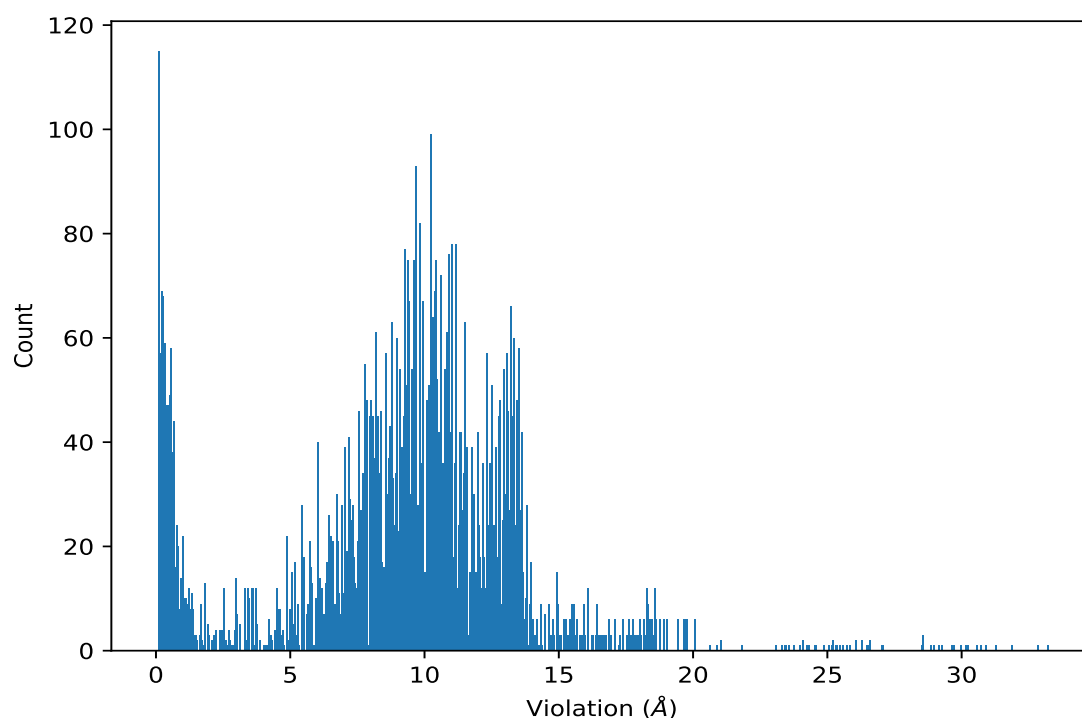
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,144)	2:1:B:MET:HE1	2:67:B:LEU:HD11	2	0.26	0.16	0.26
(3,224)	2:36:B:ILE:HA	2:71:B:LEU:HD23	2	0.26	0.08	0.26
(3,224)	2:36:B:ILE:HA	2:71:B:LEU:HD22	2	0.26	0.08	0.26
(1,3992)	2:5:B:VAL:HG13	2:7:B:THR:HG22	2	0.21	0.03	0.21
(1,3992)	2:5:B:VAL:HG11	2:7:B:THR:HG21	2	0.21	0.03	0.21
(1,4316)	2:15:B:LEU:HD12	2:29:B:LYS:HA	2	0.2	0.05	0.2
(1,4316)	2:15:B:LEU:HD22	2:29:B:LYS:HA	2	0.2	0.05	0.2
(1,1468)	2:1:C:MET:HE1	2:19:C:PRO:HG2	2	0.18	0.05	0.18
(1,1468)	2:1:C:MET:HE1	2:19:C:PRO:HG3	2	0.18	0.05	0.18
(1,1468)	2:1:C:MET:HE2	2:19:C:PRO:HG2	2	0.18	0.05	0.18
(1,1468)	2:1:C:MET:HE2	2:19:C:PRO:HG3	2	0.18	0.05	0.18
(1,1468)	2:1:C:MET:HE3	2:19:C:PRO:HG2	2	0.18	0.05	0.18
(1,1468)	2:1:C:MET:HE3	2:19:C:PRO:HG3	2	0.18	0.05	0.18
(1,5180)	2:36:B:ILE:HD11	2:71:B:LEU:HD21	2	0.18	0.02	0.18
(1,5180)	2:36:B:ILE:HD13	2:71:B:LEU:HD23	2	0.18	0.02	0.18
(1,3993)	2:5:B:VAL:HG13	2:7:B:THR:HG22	2	0.15	0.03	0.15
(1,3993)	2:5:B:VAL:HG11	2:7:B:THR:HG21	2	0.15	0.03	0.15
(1,4513)	2:52:B:ASP:HB2	2:24:B:GLU:HB2	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:504:A:GLU:OE2	2:6:C:LYS:NZ	6	33.23
(1,102)	1:504:A:GLU:OE1	2:6:C:LYS:NZ	4	32.81
(1,102)	1:504:A:GLU:OE2	2:6:C:LYS:NZ	10	31.87
(1,102)	1:504:A:GLU:OE2	2:6:C:LYS:NZ	7	31.26
(1,102)	1:504:A:GLU:OE1	2:6:C:LYS:NZ	2	30.94
(1,102)	1:504:A:GLU:OE1	2:6:C:LYS:NZ	9	30.71
(1,102)	1:504:A:GLU:OE2	2:6:C:LYS:NZ	3	30.56
(1,102)	1:504:A:GLU:OE2	2:6:C:LYS:NZ	8	30.21
(1,102)	1:504:A:GLU:OE2	2:6:C:LYS:NZ	1	30.18
(1,66)	1:583:A:ASP:OD2	2:6:B:LYS:NZ	8	29.99
(1,67)	1:592:A:GLU:OE1	2:48:B:LYS:NZ	3	29.74
(1,66)	1:583:A:ASP:OD1	2:6:B:LYS:NZ	4	29.64
(1,66)	1:583:A:ASP:OD1	2:6:B:LYS:NZ	1	29.29
(1,66)	1:583:A:ASP:OD2	2:6:B:LYS:NZ	7	29.18
(1,66)	1:583:A:ASP:OD1	2:6:B:LYS:NZ	9	28.96
(1,66)	1:583:A:ASP:OD2	2:6:B:LYS:NZ	2	28.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:583:A:ASP:OD2	2:6:B:LYS:NZ	6	28.57
(1,102)	1:504:A:GLU:OE2	2:6:C:LYS:NZ	5	28.56
(1,66)	1:583:A:ASP:OD2	2:6:B:LYS:NZ	10	28.56
(1,66)	1:583:A:ASP:OD1	2:6:B:LYS:NZ	3	28.51
(1,67)	1:592:A:GLU:OE2	2:48:B:LYS:NZ	4	27.08
(2,1)	1:583:A:ASP:OD1	2:68:B:HIS:NE2	10	27.04
(1,67)	1:592:A:GLU:OE1	2:48:B:LYS:NZ	7	26.57
(1,67)	1:592:A:GLU:OE2	2:48:B:LYS:NZ	1	26.56
(2,1)	1:583:A:ASP:OD1	2:68:B:HIS:NE2	8	26.53
(1,67)	1:592:A:GLU:OE2	2:48:B:LYS:NZ	2	26.46
(1,66)	1:583:A:ASP:OD1	2:6:B:LYS:NZ	5	26.29
(1,63)	1:541:A:ASP:OD1	2:74:B:ARG:NH2	9	26.26
(1,67)	1:592:A:GLU:OE2	2:48:B:LYS:NZ	5	26.09
(2,1)	1:583:A:ASP:OD1	2:68:B:HIS:NE2	2	26.07
(1,67)	1:592:A:GLU:OE2	2:48:B:LYS:NZ	6	25.82
(2,2)	1:583:A:ASP:OD2	2:68:B:HIS:NE2	3	25.71
(2,2)	1:583:A:ASP:OD2	2:68:B:HIS:NE2	5	25.55
(2,1)	1:583:A:ASP:OD1	2:68:B:HIS:NE2	6	25.48
(2,2)	1:583:A:ASP:OD2	2:68:B:HIS:NE2	1	25.38
(2,1)	1:583:A:ASP:OD1	2:68:B:HIS:NE2	7	25.33
(1,67)	1:592:A:GLU:OE1	2:48:B:LYS:NZ	8	25.23
(2,2)	1:583:A:ASP:OD2	2:68:B:HIS:NE2	4	25.22
(2,2)	1:583:A:ASP:OD2	2:68:B:HIS:NE2	9	25.18
(1,63)	1:541:A:ASP:OD2	2:74:B:ARG:NH2	2	25.05
(2,2)	1:583:A:ASP:OD2	2:68:B:HIS:NE2	10	24.9
(1,67)	1:592:A:GLU:OE1	2:48:B:LYS:NZ	9	24.58
(2,2)	1:583:A:ASP:OD2	2:68:B:HIS:NE2	8	24.53
(1,67)	1:592:A:GLU:OE1	2:48:B:LYS:NZ	10	24.32
(2,1)	1:583:A:ASP:OD1	2:68:B:HIS:NE2	5	24.23
(2,2)	1:583:A:ASP:OD2	2:68:B:HIS:NE2	2	24.06
(1,63)	1:541:A:ASP:OD1	2:74:B:ARG:NH2	8	24.06
(2,1)	1:583:A:ASP:OD1	2:68:B:HIS:NE2	3	23.97
(2,1)	1:583:A:ASP:OD1	2:68:B:HIS:NE2	1	23.76
(2,1)	1:583:A:ASP:OD1	2:68:B:HIS:NE2	9	23.59
(2,1)	1:583:A:ASP:OD1	2:68:B:HIS:NE2	4	23.48
(2,2)	1:583:A:ASP:OD2	2:68:B:HIS:NE2	6	23.45
(2,2)	1:583:A:ASP:OD2	2:68:B:HIS:NE2	7	23.32
(1,63)	1:541:A:ASP:OD1	2:74:B:ARG:NH1	4	23.07
(1,63)	1:541:A:ASP:OD1	2:74:B:ARG:NH1	5	21.84
(1,63)	1:541:A:ASP:OD2	2:74:B:ARG:NH2	7	21.02
(1,63)	1:541:A:ASP:OD2	2:74:B:ARG:NH1	1	21.0
(1,63)	1:541:A:ASP:OD1	2:74:B:ARG:NH2	6	20.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:541:A:ASP:OD1	2:74:B:ARG:NH2	10	20.64
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD2	3	20.09
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD3	3	20.09
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD2	3	20.09
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD3	3	20.09
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD2	3	20.09
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD3	3	20.09
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD2	1	19.77
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD3	1	19.77
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD2	1	19.77
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD3	1	19.77
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD2	1	19.77
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD3	1	19.77
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD2	10	19.73
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD3	10	19.73
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD2	10	19.73
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD3	10	19.73
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD2	10	19.73
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD3	10	19.73
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD2	9	19.7
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD3	9	19.7
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD2	9	19.7
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD3	9	19.7
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD2	9	19.7
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD3	9	19.7
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD2	6	19.43
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD3	6	19.43
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD2	6	19.43
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD3	6	19.43
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD2	6	19.43
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD3	6	19.43
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD2	8	19.01
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD3	8	19.01
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD2	8	19.01
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD3	8	19.01
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD2	8	19.01
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD3	8	19.01
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD2	5	18.92
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD3	5	18.92
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD2	5	18.92
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD3	5	18.92
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD2	5	18.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD3	5	18.92
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD2	10	18.77
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD3	10	18.77
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD2	10	18.77
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD3	10	18.77
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD2	10	18.77
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD3	10	18.77
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD2	7	18.63
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD3	7	18.63
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD2	7	18.63
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD3	7	18.63
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD2	7	18.63
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD3	7	18.63
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD2	3	18.59
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD3	3	18.59
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD2	3	18.59
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD3	3	18.59
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD2	3	18.59
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD3	3	18.59
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD2	2	18.57
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD3	2	18.57
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD2	2	18.57
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD3	2	18.57
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD2	2	18.57
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD3	2	18.57
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG21	1	18.54
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG22	1	18.54
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG23	1	18.54
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD2	1	18.46
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD3	1	18.46
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD2	1	18.46
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD3	1	18.46
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD2	1	18.46
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD3	1	18.46
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD2	2	18.41
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD3	2	18.41
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD2	2	18.41
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD3	2	18.41
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD2	2	18.41
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD3	2	18.41
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD2	4	18.36
(1,69)	1:508:A:LEU:HD21	2:6:C:LYS:HD3	4	18.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD2	4	18.36
(1,69)	1:508:A:LEU:HD22	2:6:C:LYS:HD3	4	18.36
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD2	4	18.36
(1,69)	1:508:A:LEU:HD23	2:6:C:LYS:HD3	4	18.36
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG21	10	18.32
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG22	10	18.32
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG23	10	18.32
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD2	9	18.3
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD3	9	18.3
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD2	9	18.3
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD3	9	18.3
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD2	9	18.3
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD3	9	18.3
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD2	4	18.29
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD3	4	18.29
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD2	4	18.29
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD3	4	18.29
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD2	4	18.29
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD3	4	18.29
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD2	6	18.25
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD3	6	18.25
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD2	6	18.25
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD3	6	18.25
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD2	6	18.25
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD3	6	18.25
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG21	8	18.2
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG22	8	18.2
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG23	8	18.2
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG21	3	18.18
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG22	3	18.18
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG23	3	18.18
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD11	3	18.16
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD12	3	18.16
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD13	3	18.16
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG21	7	18.09
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG22	7	18.09
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG23	7	18.09
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD11	1	18.0
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD12	1	18.0
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD13	1	18.0
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD11	10	18.0
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD12	10	18.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD13	10	18.0
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG21	5	17.97
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG22	5	17.97
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG23	5	17.97
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG21	4	17.94
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG22	4	17.94
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG23	4	17.94
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG21	2	17.83
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG22	2	17.83
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG23	2	17.83
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG21	9	17.78
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG22	9	17.78
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG23	9	17.78
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD11	7	17.78
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD12	7	17.78
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD13	7	17.78
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD11	5	17.74
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD12	5	17.74
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD13	5	17.74
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD11	4	17.68
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD12	4	17.68
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD13	4	17.68
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD2	8	17.65
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD3	8	17.65
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD2	8	17.65
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD3	8	17.65
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD2	8	17.65
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD3	8	17.65
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD11	8	17.54
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD12	8	17.54
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD13	8	17.54
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD2	5	17.37
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD3	5	17.37
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD2	5	17.37
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD3	5	17.37
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD2	5	17.37
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD3	5	17.37
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD11	2	17.25
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD12	2	17.25
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD13	2	17.25
(1,63)	1:541:A:ASP:OD1	2:74:B:ARG:NH2	3	17.24
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD2	7	17.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:508:A:LEU:HD11	2:6:C:LYS:HD3	7	17.08
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD2	7	17.08
(1,68)	1:508:A:LEU:HD12	2:6:C:LYS:HD3	7	17.08
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD2	7	17.08
(1,68)	1:508:A:LEU:HD13	2:6:C:LYS:HD3	7	17.08
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD11	9	16.93
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD12	9	16.93
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD13	9	16.93
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG21	1	16.89
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG22	1	16.89
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG23	1	16.89
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG21	3	16.89
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG22	3	16.89
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG23	3	16.89
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG21	6	16.76
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG22	6	16.76
(1,54)	1:590:A:ALA:HA	2:44:B:ILE:HG23	6	16.76
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG21	10	16.68
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG22	10	16.68
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG23	10	16.68
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG21	8	16.62
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG22	8	16.62
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG23	8	16.62
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD11	3	16.59
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD12	3	16.59
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD13	3	16.59
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG21	9	16.53
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG22	9	16.53
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG23	9	16.53
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD11	6	16.45
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD12	6	16.45
(1,53)	1:590:A:ALA:HA	2:44:B:ILE:HD13	6	16.45
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG21	4	16.44
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG22	4	16.44
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG23	4	16.44
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG21	9	16.44
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG22	9	16.44
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG23	9	16.44
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG21	7	16.43
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG22	7	16.43
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG23	7	16.43
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG21	5	16.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG22	5	16.4
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG23	5	16.4
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG21	5	16.27
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG22	5	16.27
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG23	5	16.27
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG21	1	16.23
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG22	1	16.23
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG23	1	16.23
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG21	8	16.08
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG22	8	16.08
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG23	8	16.08
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG21	1	16.07
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG22	1	16.07
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG23	1	16.07
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD11	1	16.06
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD12	1	16.06
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD13	1	16.06
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD11	10	16.06
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD12	10	16.06
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD13	10	16.06
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG21	5	15.99
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG22	5	15.99
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG23	5	15.99
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG21	4	15.95
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG22	4	15.95
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG23	4	15.95
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG21	8	15.95
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG22	8	15.95
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG23	8	15.95
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG21	3	15.9
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG22	3	15.9
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG23	3	15.9
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG21	3	15.89
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG22	3	15.89
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG23	3	15.89
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG21	10	15.85
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG22	10	15.85
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG23	10	15.85
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD11	7	15.78
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD12	7	15.78
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD13	7	15.78
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG21	7	15.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG22	7	15.65
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG23	7	15.65
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG21	7	15.65
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG22	7	15.65
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG23	7	15.65
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD11	8	15.64
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD12	8	15.64
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD13	8	15.64
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG21	2	15.6
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG22	2	15.6
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG23	2	15.6
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG21	6	15.57
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG22	6	15.57
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG23	6	15.57
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG21	4	15.55
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG22	4	15.55
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG23	4	15.55
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG21	2	15.54
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG22	2	15.54
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG23	2	15.54
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD11	1	15.52
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD12	1	15.52
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD13	1	15.52
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG21	10	15.51
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG22	10	15.51
(1,19)	1:544:A:THR:HB	2:9:B:THR:HG23	10	15.51
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD11	5	15.48
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD12	5	15.48
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD13	5	15.48
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG21	2	15.47
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG22	2	15.47
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG23	2	15.47
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG21	6	15.46
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG22	6	15.46
(1,12)	1:543:A:THR:HB	2:9:B:THR:HG23	6	15.46
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG21	9	15.45
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG22	9	15.45
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG23	9	15.45
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD11	3	15.42
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD12	3	15.42
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD13	3	15.42
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD11	10	15.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD12	10	15.35
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD13	10	15.35
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD11	5	15.27
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD12	5	15.27
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD13	5	15.27
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD11	7	15.25
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD12	7	15.25
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD13	7	15.25
(1,74)	1:508:A:LEU:HD11	2:8:C:LEU:HG	2	15.17
(1,74)	1:508:A:LEU:HD12	2:8:C:LEU:HG	2	15.17
(1,74)	1:508:A:LEU:HD13	2:8:C:LEU:HG	2	15.17
(1,74)	1:508:A:LEU:HD21	2:8:C:LEU:HG	2	15.17
(1,74)	1:508:A:LEU:HD22	2:8:C:LEU:HG	2	15.17
(1,74)	1:508:A:LEU:HD23	2:8:C:LEU:HG	2	15.17
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD11	8	15.05
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD12	8	15.05
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD13	8	15.05
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD11	4	15.01
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD12	4	15.01
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD13	4	15.01
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG21	6	14.98
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG22	6	14.98
(1,58)	1:591:A:ILE:HA	2:44:B:ILE:HG23	6	14.98
(1,74)	1:508:A:LEU:HD11	2:8:C:LEU:HG	1	14.97
(1,74)	1:508:A:LEU:HD12	2:8:C:LEU:HG	1	14.97
(1,74)	1:508:A:LEU:HD13	2:8:C:LEU:HG	1	14.97
(1,74)	1:508:A:LEU:HD21	2:8:C:LEU:HG	1	14.97
(1,74)	1:508:A:LEU:HD22	2:8:C:LEU:HG	1	14.97
(1,74)	1:508:A:LEU:HD23	2:8:C:LEU:HG	1	14.97
(1,74)	1:508:A:LEU:HD11	2:8:C:LEU:HG	5	14.92
(1,74)	1:508:A:LEU:HD12	2:8:C:LEU:HG	5	14.92
(1,74)	1:508:A:LEU:HD13	2:8:C:LEU:HG	5	14.92
(1,74)	1:508:A:LEU:HD21	2:8:C:LEU:HG	5	14.92
(1,74)	1:508:A:LEU:HD22	2:8:C:LEU:HG	5	14.92
(1,74)	1:508:A:LEU:HD23	2:8:C:LEU:HG	5	14.92
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD11	4	14.92
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD12	4	14.92
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD13	4	14.92
(1,74)	1:508:A:LEU:HD11	2:8:C:LEU:HG	3	14.91
(1,74)	1:508:A:LEU:HD12	2:8:C:LEU:HG	3	14.91
(1,74)	1:508:A:LEU:HD13	2:8:C:LEU:HG	3	14.91
(1,74)	1:508:A:LEU:HD21	2:8:C:LEU:HG	3	14.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:508:A:LEU:HD22	2:8:C:LEU:HG	3	14.91
(1,74)	1:508:A:LEU:HD23	2:8:C:LEU:HG	3	14.91
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD11	9	14.82
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD12	9	14.82
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD13	9	14.82
(1,74)	1:508:A:LEU:HD11	2:8:C:LEU:HG	4	14.76
(1,74)	1:508:A:LEU:HD12	2:8:C:LEU:HG	4	14.76
(1,74)	1:508:A:LEU:HD13	2:8:C:LEU:HG	4	14.76
(1,74)	1:508:A:LEU:HD21	2:8:C:LEU:HG	4	14.76
(1,74)	1:508:A:LEU:HD22	2:8:C:LEU:HG	4	14.76
(1,74)	1:508:A:LEU:HD23	2:8:C:LEU:HG	4	14.76
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD11	2	14.71
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD12	2	14.71
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD13	2	14.71
(1,74)	1:508:A:LEU:HD11	2:8:C:LEU:HG	7	14.63
(1,74)	1:508:A:LEU:HD12	2:8:C:LEU:HG	7	14.63
(1,74)	1:508:A:LEU:HD13	2:8:C:LEU:HG	7	14.63
(1,74)	1:508:A:LEU:HD21	2:8:C:LEU:HG	7	14.63
(1,74)	1:508:A:LEU:HD22	2:8:C:LEU:HG	7	14.63
(1,74)	1:508:A:LEU:HD23	2:8:C:LEU:HG	7	14.63
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD11	2	14.63
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD12	2	14.63
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD13	2	14.63
(1,74)	1:508:A:LEU:HD11	2:8:C:LEU:HG	9	14.48
(1,74)	1:508:A:LEU:HD12	2:8:C:LEU:HG	9	14.48
(1,74)	1:508:A:LEU:HD13	2:8:C:LEU:HG	9	14.48
(1,74)	1:508:A:LEU:HD21	2:8:C:LEU:HG	9	14.48
(1,74)	1:508:A:LEU:HD22	2:8:C:LEU:HG	9	14.48
(1,74)	1:508:A:LEU:HD23	2:8:C:LEU:HG	9	14.48
(3,11)	1:518:A:LEU:CG	2:66:C:THR:H	2	14.47
(3,11)	1:518:A:LEU:CG	2:66:C:THR:H	8	14.38
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD11	9	14.35
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD12	9	14.35
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD13	9	14.35
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD11	6	14.34
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD12	6	14.34
(1,47)	1:587:A:THR:HA	2:44:B:ILE:HD13	6	14.34
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD11	6	14.3
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD12	6	14.3
(1,57)	1:591:A:ILE:HA	2:44:B:ILE:HD13	6	14.3
(3,11)	1:518:A:LEU:CG	2:66:C:THR:H	3	14.28
(1,74)	1:508:A:LEU:HD11	2:8:C:LEU:HG	10	14.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:508:A:LEU:HD12	2:8:C:LEU:HG	10	14.17
(1,74)	1:508:A:LEU:HD13	2:8:C:LEU:HG	10	14.17
(1,74)	1:508:A:LEU:HD21	2:8:C:LEU:HG	10	14.17
(1,74)	1:508:A:LEU:HD22	2:8:C:LEU:HG	10	14.17
(1,74)	1:508:A:LEU:HD23	2:8:C:LEU:HG	10	14.17
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD11	8	14.12
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD12	8	14.12
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD13	8	14.12
(1,74)	1:508:A:LEU:HD11	2:8:C:LEU:HG	6	14.02
(1,74)	1:508:A:LEU:HD12	2:8:C:LEU:HG	6	14.02
(1,74)	1:508:A:LEU:HD13	2:8:C:LEU:HG	6	14.02
(1,74)	1:508:A:LEU:HD21	2:8:C:LEU:HG	6	14.02
(1,74)	1:508:A:LEU:HD22	2:8:C:LEU:HG	6	14.02
(1,74)	1:508:A:LEU:HD23	2:8:C:LEU:HG	6	14.02
(3,11)	1:518:A:LEU:CG	2:66:C:THR:H	1	13.98
(3,11)	1:518:A:LEU:CG	2:66:C:THR:H	5	13.98
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD21	3	13.98
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD22	3	13.98
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD23	3	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD11	5	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD12	5	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD13	5	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD21	5	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD22	5	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD23	5	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD11	10	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD12	10	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD13	10	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD21	10	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD22	10	13.98
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD23	10	13.98
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG21	1	13.92
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG22	1	13.92
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG23	1	13.92
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG21	1	13.92
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG22	1	13.92
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG23	1	13.92
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG21	1	13.92
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG22	1	13.92
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG23	1	13.92
(3,11)	1:518:A:LEU:CG	2:66:C:THR:H	10	13.86
(3,11)	1:518:A:LEU:CG	2:66:C:THR:H	6	13.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD21	1	13.83
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD22	1	13.83
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD23	1	13.83
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD21	2	13.82
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD22	2	13.82
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD23	2	13.82
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD11	1	13.82
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD12	1	13.82
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD13	1	13.82
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD21	1	13.82
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD22	1	13.82
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD23	1	13.82
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD21	4	13.81
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD22	4	13.81
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD23	4	13.81
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD21	4	13.81
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD22	4	13.81
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD23	4	13.81
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD21	4	13.81
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD22	4	13.81
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD23	4	13.81
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD11	8	13.8
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD12	8	13.8
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD13	8	13.8
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD21	8	13.8
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD22	8	13.8
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD23	8	13.8
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD21	5	13.77
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD22	5	13.77
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD23	5	13.77
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD21	5	13.77
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD22	5	13.77
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD23	5	13.77
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD21	5	13.77
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD22	5	13.77
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD23	5	13.77
(1,65)	1:552:A:GLU:OE1	2:42:B:ARG:NH1	6	13.75
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD11	7	13.74
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD12	7	13.74
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD13	7	13.74
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD21	7	13.74
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD22	7	13.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD23	7	13.74
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG21	10	13.69
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG22	10	13.69
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG23	10	13.69
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG21	10	13.69
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG22	10	13.69
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG23	10	13.69
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG21	10	13.69
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG22	10	13.69
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG23	10	13.69
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD11	3	13.67
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD12	3	13.67
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD13	3	13.67
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD21	3	13.67
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD22	3	13.67
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD23	3	13.67
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB2	8	13.63
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB3	8	13.63
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB2	8	13.63
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB3	8	13.63
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB2	8	13.63
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB3	8	13.63
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD21	4	13.63
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD22	4	13.63
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD23	4	13.63
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD11	3	13.63
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD12	3	13.63
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD13	3	13.63
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD11	3	13.63
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD12	3	13.63
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD13	3	13.63
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD11	3	13.63
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD12	3	13.63
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD13	3	13.63
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG21	8	13.63
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG22	8	13.63
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG23	8	13.63
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG21	8	13.63
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG22	8	13.63
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG23	8	13.63
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG21	8	13.63
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG22	8	13.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG23	8	13.63
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD21	6	13.63
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD22	6	13.63
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD23	6	13.63
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD21	6	13.63
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD22	6	13.63
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD23	6	13.63
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD21	6	13.63
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD22	6	13.63
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD23	6	13.63
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB2	1	13.62
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB3	1	13.62
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB2	1	13.62
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB3	1	13.62
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB2	1	13.62
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB3	1	13.62
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG21	3	13.59
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG22	3	13.59
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG23	3	13.59
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG21	3	13.59
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG22	3	13.59
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG23	3	13.59
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG21	3	13.59
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG22	3	13.59
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG23	3	13.59
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD11	10	13.58
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD12	10	13.58
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD13	10	13.58
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD11	10	13.58
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD12	10	13.58
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD13	10	13.58
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD11	10	13.58
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD12	10	13.58
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD13	10	13.58
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG21	7	13.57
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG22	7	13.57
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG23	7	13.57
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG21	7	13.57
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG22	7	13.57
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG23	7	13.57
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG21	7	13.57
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG22	7	13.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG23	7	13.57
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB2	3	13.54
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB3	3	13.54
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB2	3	13.54
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB3	3	13.54
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB2	3	13.54
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB3	3	13.54
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB2	5	13.53
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB3	5	13.53
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB2	5	13.53
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB3	5	13.53
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB2	5	13.53
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB3	5	13.53
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD11	1	13.53
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD12	1	13.53
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD13	1	13.53
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD11	1	13.53
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD12	1	13.53
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD13	1	13.53
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD11	1	13.53
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD12	1	13.53
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD13	1	13.53
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG21	4	13.53
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG22	4	13.53
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG23	4	13.53
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG21	4	13.53
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG22	4	13.53
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG23	4	13.53
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG21	4	13.53
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG22	4	13.53
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG23	4	13.53
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD11	3	13.53
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD12	3	13.53
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD13	3	13.53
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD11	3	13.53
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD12	3	13.53
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD13	3	13.53
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD11	3	13.53
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD12	3	13.53
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD13	3	13.53
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG21	2	13.52
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG22	2	13.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG23	2	13.52
(1,64)	1:548:A:ASP:OD2	2:42:B:ARG:NH2	4	13.52
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD11	6	13.52
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD12	6	13.52
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD13	6	13.52
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD21	6	13.52
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD22	6	13.52
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD23	6	13.52
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD21	10	13.5
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD22	10	13.5
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD23	10	13.5
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD21	10	13.5
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD22	10	13.5
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD23	10	13.5
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD21	10	13.5
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD22	10	13.5
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD23	10	13.5
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD11	10	13.48
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD12	10	13.48
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD13	10	13.48
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD11	10	13.48
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD12	10	13.48
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD13	10	13.48
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD11	10	13.48
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD12	10	13.48
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD13	10	13.48
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG21	5	13.48
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG22	5	13.48
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG23	5	13.48
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG21	5	13.48
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG22	5	13.48
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG23	5	13.48
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG21	5	13.48
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG22	5	13.48
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG23	5	13.48
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD21	7	13.48
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD22	7	13.48
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD23	7	13.48
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD21	7	13.48
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD22	7	13.48
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD23	7	13.48
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD21	7	13.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD22	7	13.48
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD23	7	13.48
(3,11)	1:518:A:LEU:CG	2:66:C:THR:H	7	13.47
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD21	9	13.46
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD22	9	13.46
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD23	9	13.46
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD11	5	13.46
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD12	5	13.46
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD13	5	13.46
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD11	5	13.46
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD12	5	13.46
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD13	5	13.46
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD11	5	13.46
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD12	5	13.46
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD13	5	13.46
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD21	6	13.43
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD22	6	13.43
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD23	6	13.43
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD21	6	13.43
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD22	6	13.43
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD23	6	13.43
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD21	6	13.43
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD22	6	13.43
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD23	6	13.43
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG21	2	13.42
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG22	2	13.42
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG23	2	13.42
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG21	2	13.42
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG22	2	13.42
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG23	2	13.42
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG21	2	13.42
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG22	2	13.42
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG23	2	13.42
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD11	10	13.42
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD12	10	13.42
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD13	10	13.42
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD11	10	13.42
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD12	10	13.42
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD13	10	13.42
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD11	10	13.42
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD12	10	13.42
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD13	10	13.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD11	4	13.41
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD12	4	13.41
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD13	4	13.41
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD11	4	13.41
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD12	4	13.41
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD13	4	13.41
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD11	4	13.41
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD12	4	13.41
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD13	4	13.41
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD11	5	13.4
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD12	5	13.4
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD13	5	13.4
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD11	7	13.4
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD12	7	13.4
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD13	7	13.4
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD11	7	13.4
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD12	7	13.4
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD13	7	13.4
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD11	7	13.4
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD12	7	13.4
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD13	7	13.4
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG21	9	13.39
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG22	9	13.39
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG23	9	13.39
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG21	9	13.39
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG22	9	13.39
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG23	9	13.39
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG21	9	13.39
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG22	9	13.39
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG23	9	13.39
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD11	9	13.37
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD12	9	13.37
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD13	9	13.37
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD21	9	13.37
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD22	9	13.37
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD23	9	13.37
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD11	5	13.36
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD12	5	13.36
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD13	5	13.36
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD11	5	13.36
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD12	5	13.36
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD13	5	13.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD11	5	13.36
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD12	5	13.36
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD13	5	13.36
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD21	5	13.35
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD22	5	13.35
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD23	5	13.35
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD11	7	13.35
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD12	7	13.35
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD13	7	13.35
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD11	7	13.35
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD12	7	13.35
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD13	7	13.35
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD11	7	13.35
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD12	7	13.35
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD13	7	13.35
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD11	4	13.35
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD12	4	13.35
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD13	4	13.35
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD21	4	13.35
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD22	4	13.35
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD23	4	13.35
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD21	5	13.33
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD22	5	13.33
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD23	5	13.33
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD21	5	13.33
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD22	5	13.33
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD23	5	13.33
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD21	5	13.33
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD22	5	13.33
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD23	5	13.33
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD11	2	13.33
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD12	2	13.33
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD13	2	13.33
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD21	2	13.33
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD22	2	13.33
(1,48)	1:587:A:THR:HB	2:8:B:LEU:HD23	2	13.33
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD11	1	13.33
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD12	1	13.33
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD13	1	13.33
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD11	1	13.33
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD12	1	13.33
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD13	1	13.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD11	1	13.33
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD12	1	13.33
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD13	1	13.33
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD21	5	13.32
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD22	5	13.32
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD23	5	13.32
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD21	5	13.32
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD22	5	13.32
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD23	5	13.32
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD21	5	13.32
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD22	5	13.32
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD23	5	13.32
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD21	7	13.3
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD22	7	13.3
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD23	7	13.3
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD21	7	13.3
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD22	7	13.3
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD23	7	13.3
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD21	7	13.3
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD22	7	13.3
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD23	7	13.3
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD21	10	13.28
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD22	10	13.28
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD23	10	13.28
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD21	10	13.28
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD22	10	13.28
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD23	10	13.28
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD21	10	13.28
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD22	10	13.28
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD23	10	13.28
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD11	1	13.28
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD12	1	13.28
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD13	1	13.28
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD11	1	13.28
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD12	1	13.28
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD13	1	13.28
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD11	1	13.28
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD12	1	13.28
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD13	1	13.28
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD11	10	13.27
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD12	10	13.27
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD13	10	13.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD11	10	13.27
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD12	10	13.27
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD13	10	13.27
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD11	10	13.27
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD12	10	13.27
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD13	10	13.27
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB2	9	13.26
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB3	9	13.26
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB2	9	13.26
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB3	9	13.26
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB2	9	13.26
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB3	9	13.26
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD21	8	13.26
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD22	8	13.26
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD23	8	13.26
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD21	8	13.26
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD22	8	13.26
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD23	8	13.26
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD21	8	13.26
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD22	8	13.26
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD23	8	13.26
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG21	3	13.25
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG22	3	13.25
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG23	3	13.25
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD21	7	13.23
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD22	7	13.23
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD23	7	13.23
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD21	7	13.23
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD22	7	13.23
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD23	7	13.23
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD21	7	13.23
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD22	7	13.23
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD23	7	13.23
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD11	1	13.23
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD12	1	13.23
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD13	1	13.23
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD11	1	13.23
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD12	1	13.23
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD13	1	13.23
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD11	1	13.23
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD12	1	13.23
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD13	1	13.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD21	6	13.22
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD22	6	13.22
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD23	6	13.22
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD21	6	13.22
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD22	6	13.22
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD23	6	13.22
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD21	6	13.22
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD22	6	13.22
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD23	6	13.22
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD11	7	13.22
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD12	7	13.22
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD13	7	13.22
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD11	7	13.22
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD12	7	13.22
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD13	7	13.22
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD11	7	13.22
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD12	7	13.22
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD13	7	13.22
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD21	3	13.22
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD22	3	13.22
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD23	3	13.22
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD21	3	13.22
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD22	3	13.22
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD23	3	13.22
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD21	3	13.22
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD22	3	13.22
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD23	3	13.22
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD11	5	13.22
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD12	5	13.22
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD13	5	13.22
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD11	5	13.22
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD12	5	13.22
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD13	5	13.22
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD11	5	13.22
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD12	5	13.22
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD13	5	13.22
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD21	7	13.21
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD22	7	13.21
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD23	7	13.21
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD11	8	13.21
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD12	8	13.21
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD13	8	13.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD11	8	13.21
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD12	8	13.21
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD13	8	13.21
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD11	8	13.21
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD12	8	13.21
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD13	8	13.21
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD21	3	13.2
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD22	3	13.2
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD23	3	13.2
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD21	3	13.2
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD22	3	13.2
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD23	3	13.2
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD21	3	13.2
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD22	3	13.2
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD23	3	13.2
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD11	5	13.18
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD12	5	13.18
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD13	5	13.18
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD11	5	13.18
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD12	5	13.18
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD13	5	13.18
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD11	5	13.18
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD12	5	13.18
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD13	5	13.18
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD21	2	13.17
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD22	2	13.17
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD23	2	13.17
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD21	2	13.17
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD22	2	13.17
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD23	2	13.17
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD21	2	13.17
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD22	2	13.17
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD23	2	13.17
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB2	7	13.14
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB3	7	13.14
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB2	7	13.14
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB3	7	13.14
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB2	7	13.14
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB3	7	13.14
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD11	9	13.14
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD12	9	13.14
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD13	9	13.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD11	9	13.14
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD12	9	13.14
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD13	9	13.14
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD11	9	13.14
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD12	9	13.14
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD13	9	13.14
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD11	2	13.13
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD12	2	13.13
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD13	2	13.13
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD11	8	13.13
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD12	8	13.13
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD13	8	13.13
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD11	8	13.13
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD12	8	13.13
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD13	8	13.13
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD11	8	13.13
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD12	8	13.13
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD13	8	13.13
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD11	3	13.13
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD12	3	13.13
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD13	3	13.13
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD11	3	13.13
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD12	3	13.13
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD13	3	13.13
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD11	3	13.13
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD12	3	13.13
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD13	3	13.13
(3,11)	1:518:A:LEU:CG	2:66:C:THR:H	4	13.11
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD21	4	13.11
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD22	4	13.11
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD23	4	13.11
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD21	4	13.11
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD22	4	13.11
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD23	4	13.11
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD21	4	13.11
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD22	4	13.11
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD23	4	13.11
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG21	5	13.1
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG22	5	13.1
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG23	5	13.1
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD21	1	13.09
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD22	1	13.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD23	1	13.09
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD21	1	13.09
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD22	1	13.09
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD23	1	13.09
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD21	1	13.09
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD22	1	13.09
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD23	1	13.09
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD21	8	13.09
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD22	8	13.09
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD23	8	13.09
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD21	8	13.09
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD22	8	13.09
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD23	8	13.09
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD21	8	13.09
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD22	8	13.09
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD23	8	13.09
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD21	9	13.09
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD22	9	13.09
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD23	9	13.09
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD21	9	13.09
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD22	9	13.09
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD23	9	13.09
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD21	9	13.09
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD22	9	13.09
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD23	9	13.09
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD21	8	13.08
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD22	8	13.08
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD23	8	13.08
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD21	8	13.08
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD22	8	13.08
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD23	8	13.08
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD21	8	13.08
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD22	8	13.08
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD23	8	13.08
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD21	5	13.07
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD22	5	13.07
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD23	5	13.07
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD21	5	13.07
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD22	5	13.07
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD23	5	13.07
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD21	5	13.07
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD22	5	13.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD23	5	13.07
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG21	7	13.06
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG22	7	13.06
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG23	7	13.06
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB2	2	13.06
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB3	2	13.06
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB2	2	13.06
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB3	2	13.06
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB2	2	13.06
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB3	2	13.06
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG21	8	13.04
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG22	8	13.04
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG23	8	13.04
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD11	6	13.03
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD12	6	13.03
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD13	6	13.03
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD11	6	13.03
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD12	6	13.03
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD13	6	13.03
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD11	6	13.03
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD12	6	13.03
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD13	6	13.03
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD11	2	13.02
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD12	2	13.02
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD13	2	13.02
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD11	2	13.02
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD12	2	13.02
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD13	2	13.02
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD11	2	13.02
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD12	2	13.02
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD13	2	13.02
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD21	1	13.0
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD22	1	13.0
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD23	1	13.0
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD21	1	13.0
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD22	1	13.0
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD23	1	13.0
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD21	1	13.0
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD22	1	13.0
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD23	1	13.0
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD11	1	12.99
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD12	1	12.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD13	1	12.99
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD11	1	12.99
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD12	1	12.99
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD13	1	12.99
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD11	1	12.99
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD12	1	12.99
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD13	1	12.99
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD21	10	12.98
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD22	10	12.98
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD23	10	12.98
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD21	10	12.98
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD22	10	12.98
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD23	10	12.98
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD21	10	12.98
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD22	10	12.98
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD23	10	12.98
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD11	5	12.98
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD12	5	12.98
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD13	5	12.98
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD11	5	12.98
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD12	5	12.98
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD13	5	12.98
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD11	5	12.98
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD12	5	12.98
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD13	5	12.98
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD21	6	12.97
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD22	6	12.97
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD23	6	12.97
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD21	6	12.97
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD22	6	12.97
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD23	6	12.97
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD21	6	12.97
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD22	6	12.97
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD23	6	12.97
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD21	3	12.96
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD22	3	12.96
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD23	3	12.96
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD21	3	12.96
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD22	3	12.96
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD23	3	12.96
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD21	3	12.96
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD22	3	12.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD23	3	12.96
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD11	9	12.96
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD12	9	12.96
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD13	9	12.96
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD11	9	12.96
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD12	9	12.96
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD13	9	12.96
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD11	9	12.96
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD12	9	12.96
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD13	9	12.96
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD21	10	12.95
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD22	10	12.95
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD23	10	12.95
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD21	10	12.94
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD22	10	12.94
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD23	10	12.94
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD21	10	12.94
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD22	10	12.94
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD23	10	12.94
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD21	10	12.94
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD22	10	12.94
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD23	10	12.94
(3,11)	1:518:A:LEU:CG	2:66:C:THR:H	9	12.92
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD11	1	12.9
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD12	1	12.9
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD13	1	12.9
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD21	2	12.9
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD22	2	12.9
(1,46)	1:584:A:VAL:HG21	2:8:B:LEU:HD23	2	12.9
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD21	2	12.9
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD22	2	12.9
(1,46)	1:584:A:VAL:HG22	2:8:B:LEU:HD23	2	12.9
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD21	2	12.9
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD22	2	12.9
(1,46)	1:584:A:VAL:HG23	2:8:B:LEU:HD23	2	12.9
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD11	4	12.88
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD12	4	12.88
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD13	4	12.88
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD11	4	12.88
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD12	4	12.88
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD13	4	12.88
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD11	4	12.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD12	4	12.88
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD13	4	12.88
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD11	8	12.83
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD12	8	12.83
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD13	8	12.83
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD11	8	12.83
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD12	8	12.83
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD13	8	12.83
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD11	8	12.83
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD12	8	12.83
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD13	8	12.83
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD11	9	12.82
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD12	9	12.82
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD13	9	12.82
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD11	9	12.82
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD12	9	12.82
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD13	9	12.82
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD11	9	12.82
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD12	9	12.82
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD13	9	12.82
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD11	8	12.82
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD12	8	12.82
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD13	8	12.82
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD11	8	12.82
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD12	8	12.82
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD13	8	12.82
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD11	8	12.82
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD12	8	12.82
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD13	8	12.82
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB2	10	12.81
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB3	10	12.81
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB2	10	12.81
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB3	10	12.81
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB2	10	12.81
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB3	10	12.81
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD11	2	12.81
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD12	2	12.81
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD13	2	12.81
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD11	2	12.81
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD12	2	12.81
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD13	2	12.81
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD11	2	12.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD12	2	12.81
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD13	2	12.81
(1,74)	1:508:A:LEU:HD11	2:8:C:LEU:HG	8	12.8
(1,74)	1:508:A:LEU:HD12	2:8:C:LEU:HG	8	12.8
(1,74)	1:508:A:LEU:HD13	2:8:C:LEU:HG	8	12.8
(1,74)	1:508:A:LEU:HD21	2:8:C:LEU:HG	8	12.8
(1,74)	1:508:A:LEU:HD22	2:8:C:LEU:HG	8	12.8
(1,74)	1:508:A:LEU:HD23	2:8:C:LEU:HG	8	12.8
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD11	3	12.79
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD12	3	12.79
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD13	3	12.79
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD11	4	12.79
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD12	4	12.79
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD13	4	12.79
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD11	4	12.79
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD12	4	12.79
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD13	4	12.79
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD11	4	12.79
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD12	4	12.79
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD13	4	12.79
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD21	4	12.77
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD22	4	12.77
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD23	4	12.77
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD21	4	12.77
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD22	4	12.77
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD23	4	12.77
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD21	4	12.77
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD22	4	12.77
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD23	4	12.77
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD11	9	12.77
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD12	9	12.77
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD13	9	12.77
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD11	9	12.77
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD12	9	12.77
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD13	9	12.77
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD11	9	12.77
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD12	9	12.77
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD13	9	12.77
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG21	4	12.76
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG22	4	12.76
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG23	4	12.76
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD11	9	12.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD12	9	12.76
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD13	9	12.76
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD11	9	12.76
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD12	9	12.76
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD13	9	12.76
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD11	9	12.76
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD12	9	12.76
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD13	9	12.76
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD11	7	12.75
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD12	7	12.75
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD13	7	12.75
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD11	6	12.74
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD12	6	12.74
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD13	6	12.74
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD11	6	12.74
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD12	6	12.74
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD13	6	12.74
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD11	6	12.74
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD12	6	12.74
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD13	6	12.74
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD11	4	12.73
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD12	4	12.73
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD13	4	12.73
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB2	4	12.72
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB3	4	12.72
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB2	4	12.72
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB3	4	12.72
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB2	4	12.72
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB3	4	12.72
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB2	6	12.67
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB3	6	12.67
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB2	6	12.67
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB3	6	12.67
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB2	6	12.67
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB3	6	12.67
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD21	9	12.67
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD22	9	12.67
(1,50)	1:587:A:THR:HG21	2:8:B:LEU:HD23	9	12.67
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD21	9	12.67
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD22	9	12.67
(1,50)	1:587:A:THR:HG22	2:8:B:LEU:HD23	9	12.67
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD21	9	12.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD22	9	12.67
(1,50)	1:587:A:THR:HG23	2:8:B:LEU:HD23	9	12.67
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD11	3	12.67
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD12	3	12.67
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD13	3	12.67
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD11	3	12.67
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD12	3	12.67
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD13	3	12.67
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD11	3	12.67
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD12	3	12.67
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD13	3	12.67
(1,20)	1:544:A:THR:HG21	2:8:B:LEU:HA	8	12.67
(1,20)	1:544:A:THR:HG22	2:8:B:LEU:HA	8	12.67
(1,20)	1:544:A:THR:HG23	2:8:B:LEU:HA	8	12.67
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG21	1	12.66
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG22	1	12.66
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG23	1	12.66
(1,20)	1:544:A:THR:HG21	2:8:B:LEU:HA	1	12.66
(1,20)	1:544:A:THR:HG22	2:8:B:LEU:HA	1	12.66
(1,20)	1:544:A:THR:HG23	2:8:B:LEU:HA	1	12.66
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB2	2	12.65
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB3	2	12.65
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB2	2	12.65
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB3	2	12.65
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB2	2	12.65
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB3	2	12.65
(1,20)	1:544:A:THR:HG21	2:8:B:LEU:HA	3	12.63
(1,20)	1:544:A:THR:HG22	2:8:B:LEU:HA	3	12.63
(1,20)	1:544:A:THR:HG23	2:8:B:LEU:HA	3	12.63
(1,20)	1:544:A:THR:HG21	2:8:B:LEU:HA	5	12.63
(1,20)	1:544:A:THR:HG22	2:8:B:LEU:HA	5	12.63
(1,20)	1:544:A:THR:HG23	2:8:B:LEU:HA	5	12.63
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD21	1	12.59
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD22	1	12.59
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD23	1	12.59
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD21	1	12.59
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD22	1	12.59
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD23	1	12.59
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD21	1	12.59
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD22	1	12.59
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD23	1	12.59
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD21	6	12.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD22	6	12.58
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD23	6	12.58
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD11	2	12.58
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD12	2	12.58
(1,44)	1:584:A:VAL:HG21	2:8:B:LEU:HD13	2	12.58
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD11	2	12.58
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD12	2	12.58
(1,44)	1:584:A:VAL:HG22	2:8:B:LEU:HD13	2	12.58
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD11	2	12.58
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD12	2	12.58
(1,44)	1:584:A:VAL:HG23	2:8:B:LEU:HD13	2	12.58
(1,20)	1:544:A:THR:HG21	2:8:B:LEU:HA	7	12.56
(1,20)	1:544:A:THR:HG22	2:8:B:LEU:HA	7	12.56
(1,20)	1:544:A:THR:HG23	2:8:B:LEU:HA	7	12.56
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD21	8	12.54
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD22	8	12.54
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD23	8	12.54
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD21	8	12.54
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD22	8	12.54
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD23	8	12.54
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD21	8	12.54
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD22	8	12.54
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD23	8	12.54
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD11	6	12.52
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD12	6	12.52
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD13	6	12.52
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD11	6	12.52
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD12	6	12.52
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD13	6	12.52
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD11	6	12.52
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD12	6	12.52
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD13	6	12.52
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB2	4	12.51
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB3	4	12.51
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB2	4	12.51
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB3	4	12.51
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB2	4	12.51
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB3	4	12.51
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD21	9	12.51
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD22	9	12.51
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD23	9	12.51
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD21	9	12.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD22	9	12.51
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD23	9	12.51
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD21	9	12.51
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD22	9	12.51
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD23	9	12.51
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD11	10	12.51
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD12	10	12.51
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD13	10	12.51
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD11	10	12.51
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD12	10	12.51
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD13	10	12.51
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD11	10	12.51
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD12	10	12.51
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD13	10	12.51
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD11	8	12.5
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD12	8	12.5
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD13	8	12.5
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD11	8	12.5
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD12	8	12.5
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD13	8	12.5
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD11	8	12.5
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD12	8	12.5
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD13	8	12.5
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG21	10	12.49
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG22	10	12.49
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG23	10	12.49
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG21	6	12.48
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG22	6	12.48
(1,55)	1:590:A:ALA:HB1	2:44:B:ILE:HG23	6	12.48
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG21	6	12.48
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG22	6	12.48
(1,55)	1:590:A:ALA:HB2	2:44:B:ILE:HG23	6	12.48
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG21	6	12.48
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG22	6	12.48
(1,55)	1:590:A:ALA:HB3	2:44:B:ILE:HG23	6	12.48
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD11	2	12.47
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD12	2	12.47
(1,49)	1:587:A:THR:HG21	2:8:B:LEU:HD13	2	12.47
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD11	2	12.47
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD12	2	12.47
(1,49)	1:587:A:THR:HG22	2:8:B:LEU:HD13	2	12.47
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD11	2	12.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD12	2	12.47
(1,49)	1:587:A:THR:HG23	2:8:B:LEU:HD13	2	12.47
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD21	5	12.46
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD22	5	12.46
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD23	5	12.46
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD11	7	12.45
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD12	7	12.45
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD13	7	12.45
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD11	7	12.45
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD12	7	12.45
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD13	7	12.45
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD11	7	12.45
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD12	7	12.45
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD13	7	12.45
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD11	8	12.44
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD12	8	12.44
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD13	8	12.44
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD11	6	12.42
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD12	6	12.42
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD13	6	12.42
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD11	7	12.42
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD12	7	12.42
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD13	7	12.42
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD11	7	12.42
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD12	7	12.42
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD13	7	12.42
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD11	7	12.42
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD12	7	12.42
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD13	7	12.42
(1,20)	1:544:A:THR:HG21	2:8:B:LEU:HA	4	12.42
(1,20)	1:544:A:THR:HG22	2:8:B:LEU:HA	4	12.42
(1,20)	1:544:A:THR:HG23	2:8:B:LEU:HA	4	12.42
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD11	4	12.4
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD12	4	12.4
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD13	4	12.4
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD11	4	12.4
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD12	4	12.4
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD13	4	12.4
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD11	4	12.4
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD12	4	12.4
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD13	4	12.4
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD21	3	12.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD22	3	12.39
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD23	3	12.39
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD21	3	12.39
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD22	3	12.39
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD23	3	12.39
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD21	3	12.39
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD22	3	12.39
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD23	3	12.39
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD21	4	12.39
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD22	4	12.39
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD23	4	12.39
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD21	4	12.39
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD22	4	12.39
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD23	4	12.39
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD21	4	12.39
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD22	4	12.39
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD23	4	12.39
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	3	12.36
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	3	12.36
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	3	12.36
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	3	12.36
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	3	12.36
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	3	12.36
(1,20)	1:544:A:THR:HG21	2:8:B:LEU:HA	9	12.34
(1,20)	1:544:A:THR:HG22	2:8:B:LEU:HA	9	12.34
(1,20)	1:544:A:THR:HG23	2:8:B:LEU:HA	9	12.34
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD21	2	12.33
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD22	2	12.33
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD23	2	12.33
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD21	2	12.33
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD22	2	12.33
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD23	2	12.33
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD21	2	12.33
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD22	2	12.33
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD23	2	12.33
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD11	3	12.33
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD12	3	12.33
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD13	3	12.33
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD11	3	12.33
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD12	3	12.33
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD13	3	12.33
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD11	3	12.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD12	3	12.33
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD13	3	12.33
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD21	7	12.32
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD22	7	12.32
(1,45)	1:584:A:VAL:HG11	2:8:B:LEU:HD23	7	12.32
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD21	7	12.32
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD22	7	12.32
(1,45)	1:584:A:VAL:HG12	2:8:B:LEU:HD23	7	12.32
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD21	7	12.32
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD22	7	12.32
(1,45)	1:584:A:VAL:HG13	2:8:B:LEU:HD23	7	12.32
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD11	6	12.31
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD12	6	12.31
(1,56)	1:590:A:ALA:HB1	2:44:B:ILE:HD13	6	12.31
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD11	6	12.31
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD12	6	12.31
(1,56)	1:590:A:ALA:HB2	2:44:B:ILE:HD13	6	12.31
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD11	6	12.31
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD12	6	12.31
(1,56)	1:590:A:ALA:HB3	2:44:B:ILE:HD13	6	12.31
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD11	4	12.31
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD12	4	12.31
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD13	4	12.31
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD11	4	12.31
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD12	4	12.31
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD13	4	12.31
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD11	4	12.31
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD12	4	12.31
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD13	4	12.31
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB2	1	12.3
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB3	1	12.3
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB2	1	12.3
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB3	1	12.3
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB2	1	12.3
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB3	1	12.3
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD21	8	12.3
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD22	8	12.3
(1,71)	1:508:A:LEU:HA	2:8:C:LEU:HD23	8	12.3
(1,20)	1:544:A:THR:HG21	2:8:B:LEU:HA	10	12.29
(1,20)	1:544:A:THR:HG22	2:8:B:LEU:HA	10	12.29
(1,20)	1:544:A:THR:HG23	2:8:B:LEU:HA	10	12.29
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD11	9	12.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD12	9	12.28
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD13	9	12.28
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD21	6	12.28
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD22	6	12.28
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD23	6	12.28
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD21	10	12.25
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD22	10	12.25
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD23	10	12.25
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD11	5	12.24
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD12	5	12.24
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD13	5	12.24
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD21	5	12.24
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD22	5	12.24
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD23	5	12.24
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD21	4	12.23
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD22	4	12.23
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD23	4	12.23
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG21	10	12.22
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG22	10	12.22
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG23	10	12.22
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG21	10	12.22
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG22	10	12.22
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG23	10	12.22
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG21	10	12.22
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG22	10	12.22
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG23	10	12.22
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG21	1	12.2
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG22	1	12.2
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG23	1	12.2
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG21	1	12.2
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG22	1	12.2
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG23	1	12.2
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG21	1	12.2
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG22	1	12.2
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG23	1	12.2
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD21	3	12.2
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD22	3	12.2
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD23	3	12.2
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB2	8	12.19
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB3	8	12.19
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB2	8	12.19
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB3	8	12.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB2	8	12.19
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB3	8	12.19
(1,20)	1:544:A:THR:HG21	2:8:B:LEU:HA	2	12.18
(1,20)	1:544:A:THR:HG22	2:8:B:LEU:HA	2	12.18
(1,20)	1:544:A:THR:HG23	2:8:B:LEU:HA	2	12.18
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD21	7	12.18
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD22	7	12.18
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD23	7	12.18
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD21	9	12.18
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD22	9	12.18
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD23	9	12.18
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG21	3	12.16
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG22	3	12.16
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG23	3	12.16
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG21	3	12.16
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG22	3	12.16
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG23	3	12.16
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG21	3	12.16
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG22	3	12.16
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG23	3	12.16
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD21	1	12.14
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD22	1	12.14
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD23	1	12.14
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD11	10	12.12
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD12	10	12.12
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD13	10	12.12
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD11	8	12.12
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD12	8	12.12
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD13	8	12.12
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD21	8	12.12
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD22	8	12.12
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD23	8	12.12
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD21	3	12.1
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD22	3	12.1
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD23	3	12.1
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG21	10	12.09
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG22	10	12.09
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG23	10	12.09
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG21	10	12.09
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG22	10	12.09
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG23	10	12.09
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG21	10	12.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG22	10	12.09
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG23	10	12.09
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD11	10	12.08
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD12	10	12.08
(1,70)	1:508:A:LEU:HA	2:8:C:LEU:HD13	10	12.08
(1,20)	1:544:A:THR:HG21	2:8:B:LEU:HA	6	12.07
(1,20)	1:544:A:THR:HG22	2:8:B:LEU:HA	6	12.07
(1,20)	1:544:A:THR:HG23	2:8:B:LEU:HA	6	12.07
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB2	3	12.03
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB3	3	12.03
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB2	3	12.03
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB3	3	12.03
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB2	3	12.03
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB3	3	12.03
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD11	6	12.03
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD12	6	12.03
(1,31)	1:544:A:THR:HG21	2:71:B:LEU:HD13	6	12.03
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD11	6	12.03
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD12	6	12.03
(1,31)	1:544:A:THR:HG22	2:71:B:LEU:HD13	6	12.03
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD11	6	12.03
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD12	6	12.03
(1,31)	1:544:A:THR:HG23	2:71:B:LEU:HD13	6	12.03
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD11	1	12.03
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD12	1	12.03
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD13	1	12.03
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	5	12.02
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	5	12.02
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	5	12.02
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	5	12.02
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	5	12.02
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	5	12.02
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD21	1	11.99
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD22	1	11.99
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD23	1	11.99
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD21	1	11.99
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD22	1	11.99
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD23	1	11.99
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD21	1	11.99
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD22	1	11.99
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD23	1	11.99
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	1	11.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	1	11.99
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	1	11.99
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	1	11.99
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	1	11.99
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	1	11.99
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB2	5	11.97
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB3	5	11.97
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB2	5	11.97
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB3	5	11.97
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB2	5	11.97
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB3	5	11.97
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG21	5	11.97
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG22	5	11.97
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG23	5	11.97
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG21	5	11.97
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG22	5	11.97
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG23	5	11.97
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG21	5	11.97
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG22	5	11.97
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG23	5	11.97
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD21	8	11.97
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD22	8	11.97
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD23	8	11.97
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD11	3	11.96
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD12	3	11.96
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD13	3	11.96
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD11	3	11.96
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD12	3	11.96
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD13	3	11.96
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD11	3	11.96
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD12	3	11.96
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD13	3	11.96
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG21	8	11.95
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG22	8	11.95
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG23	8	11.95
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG21	8	11.95
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG22	8	11.95
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG23	8	11.95
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG21	8	11.95
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG22	8	11.95
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG23	8	11.95
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD11	3	11.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD12	3	11.93
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD13	3	11.93
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD21	3	11.93
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD22	3	11.93
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD23	3	11.93
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD11	5	11.89
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD12	5	11.89
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD13	5	11.89
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD11	9	11.87
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD12	9	11.87
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD13	9	11.87
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB2	9	11.84
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB3	9	11.84
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB2	9	11.84
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB3	9	11.84
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB2	9	11.84
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB3	9	11.84
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG21	2	11.84
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG22	2	11.84
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG23	2	11.84
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG21	2	11.84
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG22	2	11.84
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG23	2	11.84
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG21	2	11.84
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG22	2	11.84
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG23	2	11.84
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG21	7	11.81
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG22	7	11.81
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG23	7	11.81
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG21	7	11.81
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG22	7	11.81
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG23	7	11.81
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG21	7	11.81
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG22	7	11.81
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG23	7	11.81
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD11	6	11.81
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD12	6	11.81
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD13	6	11.81
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG21	6	11.8
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG22	6	11.8
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG23	6	11.8
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD11	2	11.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD12	2	11.78
(1,43)	1:584:A:VAL:HG11	2:8:B:LEU:HD13	2	11.78
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD11	2	11.78
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD12	2	11.78
(1,43)	1:584:A:VAL:HG12	2:8:B:LEU:HD13	2	11.78
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD11	2	11.78
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD12	2	11.78
(1,43)	1:584:A:VAL:HG13	2:8:B:LEU:HD13	2	11.78
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD21	9	11.78
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD22	9	11.78
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD23	9	11.78
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD21	9	11.78
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD22	9	11.78
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD23	9	11.78
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD21	9	11.78
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD22	9	11.78
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD23	9	11.78
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG21	1	11.77
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG22	1	11.77
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG23	1	11.77
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG21	1	11.77
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG22	1	11.77
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG23	1	11.77
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG21	1	11.77
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG22	1	11.77
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG23	1	11.77
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD11	5	11.76
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD12	5	11.76
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD13	5	11.76
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG21	9	11.75
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG22	9	11.75
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG23	9	11.75
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG21	9	11.75
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG22	9	11.75
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG23	9	11.75
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG21	9	11.75
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG22	9	11.75
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG23	9	11.75
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD11	7	11.74
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD12	7	11.74
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD13	7	11.74
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD11	8	11.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD12	8	11.7
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD13	8	11.7
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD11	8	11.7
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD12	8	11.7
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD13	8	11.7
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD11	8	11.7
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD12	8	11.7
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD13	8	11.7
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB2	10	11.69
(1,73)	1:508:A:LEU:HD21	2:8:C:LEU:HB3	10	11.69
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB2	10	11.69
(1,73)	1:508:A:LEU:HD22	2:8:C:LEU:HB3	10	11.69
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB2	10	11.69
(1,73)	1:508:A:LEU:HD23	2:8:C:LEU:HB3	10	11.69
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD21	2	11.63
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD22	2	11.63
(1,11)	1:543:A:THR:HB	2:8:B:LEU:HD23	2	11.63
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	8	11.58
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	8	11.58
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	8	11.58
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	8	11.58
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	8	11.58
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	8	11.58
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD11	4	11.58
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD12	4	11.58
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD13	4	11.58
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB2	7	11.57
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB3	7	11.57
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB2	7	11.57
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB3	7	11.57
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB2	7	11.57
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB3	7	11.57
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD11	10	11.56
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD12	10	11.56
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD13	10	11.56
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD11	10	11.56
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD12	10	11.56
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD13	10	11.56
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD11	10	11.56
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD12	10	11.56
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD13	10	11.56
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG21	7	11.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG22	7	11.56
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG23	7	11.56
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG21	7	11.56
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG22	7	11.56
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG23	7	11.56
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG21	7	11.56
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG22	7	11.56
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG23	7	11.56
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD21	5	11.56
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD22	5	11.56
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD23	5	11.56
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG21	9	11.55
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG22	9	11.55
(1,92)	1:515:A:SER:HA	2:44:C:ILE:HG23	9	11.55
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD21	3	11.54
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD22	3	11.54
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD23	3	11.54
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD21	3	11.54
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD22	3	11.54
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD23	3	11.54
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD21	3	11.54
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD22	3	11.54
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD23	3	11.54
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD11	1	11.54
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD12	1	11.54
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD13	1	11.54
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD11	1	11.54
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD12	1	11.54
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD13	1	11.54
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD11	1	11.54
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD12	1	11.54
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD13	1	11.54
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD21	2	11.54
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD22	2	11.54
(1,32)	1:544:A:THR:HG21	2:71:B:LEU:HD23	2	11.54
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD21	2	11.54
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD22	2	11.54
(1,32)	1:544:A:THR:HG22	2:71:B:LEU:HD23	2	11.54
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD21	2	11.54
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD22	2	11.54
(1,32)	1:544:A:THR:HG23	2:71:B:LEU:HD23	2	11.54
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG21	4	11.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG22	4	11.53
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG23	4	11.53
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG21	4	11.53
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG22	4	11.53
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG23	4	11.53
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG21	4	11.53
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG22	4	11.53
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG23	4	11.53
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG21	10	11.53
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG22	10	11.53
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG23	10	11.53
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG21	10	11.53
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG22	10	11.53
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG23	10	11.53
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG21	10	11.53
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG22	10	11.53
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG23	10	11.53
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD11	2	11.53
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD12	2	11.53
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD13	2	11.53
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG21	1	11.5
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG22	1	11.5
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG23	1	11.5
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG21	1	11.5
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG22	1	11.5
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG23	1	11.5
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG21	1	11.5
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG22	1	11.5
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG23	1	11.5
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	9	11.5
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	9	11.5
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	9	11.5
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	9	11.5
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	9	11.5
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	9	11.5
(3,12)	1:518:A:LEU:CG	2:67:C:LEU:H	8	11.49
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD11	10	11.49
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD12	10	11.49
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD13	10	11.49
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD11	10	11.49
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD12	10	11.49
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD13	10	11.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD11	10	11.49
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD12	10	11.49
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD13	10	11.49
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG21	3	11.48
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG22	3	11.48
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG23	3	11.48
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG21	3	11.48
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG22	3	11.48
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG23	3	11.48
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG21	3	11.48
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG22	3	11.48
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG23	3	11.48
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD11	2	11.47
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD12	2	11.47
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD13	2	11.47
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD11	2	11.47
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD12	2	11.47
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD13	2	11.47
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG21	5	11.47
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG22	5	11.47
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG23	5	11.47
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG21	5	11.47
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG22	5	11.47
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG23	5	11.47
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG21	5	11.47
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG22	5	11.47
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG23	5	11.47
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG21	8	11.44
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG22	8	11.44
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG23	8	11.44
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG21	8	11.44
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG22	8	11.44
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG23	8	11.44
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG21	8	11.44
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG22	8	11.44
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG23	8	11.44
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG21	3	11.41
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG22	3	11.41
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG23	3	11.41
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG21	3	11.41
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG22	3	11.41
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG23	3	11.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG21	3	11.41
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG22	3	11.41
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG23	3	11.41
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	2	11.41
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	2	11.41
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	2	11.41
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	2	11.41
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	2	11.41
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	2	11.41
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD11	8	11.4
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD12	8	11.4
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD13	8	11.4
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD11	5	11.39
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD12	5	11.39
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD13	5	11.39
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD11	5	11.39
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD12	5	11.39
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD13	5	11.39
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD11	5	11.39
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD12	5	11.39
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD13	5	11.39
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD11	5	11.38
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD12	5	11.38
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD13	5	11.38
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD11	5	11.38
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD12	5	11.38
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD13	5	11.38
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB2	6	11.37
(1,72)	1:508:A:LEU:HD11	2:8:C:LEU:HB3	6	11.37
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB2	6	11.37
(1,72)	1:508:A:LEU:HD12	2:8:C:LEU:HB3	6	11.37
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB2	6	11.37
(1,72)	1:508:A:LEU:HD13	2:8:C:LEU:HB3	6	11.37
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG21	9	11.37
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG22	9	11.37
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG23	9	11.37
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG21	9	11.37
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG22	9	11.37
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG23	9	11.37
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG21	9	11.37
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG22	9	11.37
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG23	9	11.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD11	1	11.36
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD12	1	11.36
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD13	1	11.36
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD11	1	11.36
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD12	1	11.36
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD13	1	11.36
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB2	6	11.36
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB3	6	11.36
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB2	6	11.36
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB3	6	11.36
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB2	6	11.36
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB3	6	11.36
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD11	3	11.35
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD12	3	11.35
(1,10)	1:543:A:THR:HB	2:8:B:LEU:HD13	3	11.35
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD21	2	11.34
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD22	2	11.34
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD23	2	11.34
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD21	2	11.34
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD22	2	11.34
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD23	2	11.34
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD21	2	11.34
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD22	2	11.34
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD23	2	11.34
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG11	7	11.34
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG12	7	11.34
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG13	7	11.34
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG11	7	11.34
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG12	7	11.34
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG13	7	11.34
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG11	7	11.34
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG12	7	11.34
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG13	7	11.34
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD11	10	11.33
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD12	10	11.33
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD13	10	11.33
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD11	10	11.33
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD12	10	11.33
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD13	10	11.33
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD11	3	11.32
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD12	3	11.32
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD13	3	11.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD11	3	11.32
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD12	3	11.32
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD13	3	11.32
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD11	7	11.32
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD12	7	11.32
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD13	7	11.32
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD11	7	11.32
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD12	7	11.32
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD13	7	11.32
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD11	7	11.32
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD12	7	11.32
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD13	7	11.32
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD11	4	11.29
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD12	4	11.29
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD13	4	11.29
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD11	4	11.29
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD12	4	11.29
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD13	4	11.29
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD21	8	11.27
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD22	8	11.27
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD23	8	11.27
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD21	1	11.26
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD22	1	11.26
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD23	1	11.26
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD21	1	11.26
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD22	1	11.26
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD23	1	11.26
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD21	1	11.26
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD22	1	11.26
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD23	1	11.26
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD21	3	11.25
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD22	3	11.25
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD23	3	11.25
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD21	7	11.25
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD22	7	11.25
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD23	7	11.25
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD11	7	11.24
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD12	7	11.24
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD13	7	11.24
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD11	7	11.24
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD12	7	11.24
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD13	7	11.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	10	11.21
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	10	11.21
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	10	11.21
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	10	11.21
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	10	11.21
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	10	11.21
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD11	8	11.2
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD12	8	11.2
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD13	8	11.2
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD11	8	11.2
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD12	8	11.2
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD13	8	11.2
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD11	8	11.2
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD12	8	11.2
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD13	8	11.2
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD11	8	11.2
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD12	8	11.2
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD13	8	11.2
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD11	8	11.2
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD12	8	11.2
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD13	8	11.2
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD11	8	11.2
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD12	8	11.2
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD13	8	11.2
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG11	5	11.2
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG12	5	11.2
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG13	5	11.2
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG11	5	11.2
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG12	5	11.2
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG13	5	11.2
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG11	5	11.2
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG12	5	11.2
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG13	5	11.2
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD11	8	11.19
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD12	8	11.19
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD13	8	11.19
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD11	8	11.19
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD12	8	11.19
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD13	8	11.19
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD11	8	11.19
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD12	8	11.19
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD13	8	11.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG11	3	11.18
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG12	3	11.18
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG13	3	11.18
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG11	3	11.18
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG12	3	11.18
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG13	3	11.18
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG11	3	11.18
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG12	3	11.18
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG13	3	11.18
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD21	7	11.17
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD22	7	11.17
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD23	7	11.17
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD21	7	11.17
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD22	7	11.17
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD23	7	11.17
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD21	7	11.17
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD22	7	11.17
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD23	7	11.17
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD21	4	11.16
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD22	4	11.16
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD23	4	11.16
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD21	4	11.16
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD22	4	11.16
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD23	4	11.16
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD21	4	11.16
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD22	4	11.16
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD23	4	11.16
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG21	7	11.16
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG22	7	11.16
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG23	7	11.16
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG21	7	11.16
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG22	7	11.16
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG23	7	11.16
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG21	7	11.16
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG22	7	11.16
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG23	7	11.16
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	7	11.15
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	7	11.15
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	7	11.15
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	7	11.15
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	7	11.15
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	7	11.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG21	2	11.14
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG22	2	11.14
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG23	2	11.14
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG21	2	11.14
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG22	2	11.14
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG23	2	11.14
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG21	4	11.14
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG22	4	11.14
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG23	4	11.14
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG21	4	11.14
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG22	4	11.14
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG23	4	11.14
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG21	4	11.14
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG22	4	11.14
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG23	4	11.14
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD21	1	11.14
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD22	1	11.14
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD23	1	11.14
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD11	8	11.12
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD12	8	11.12
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD13	8	11.12
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD11	8	11.12
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD12	8	11.12
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD13	8	11.12
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG11	10	11.12
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG12	10	11.12
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG13	10	11.12
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG11	10	11.12
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG12	10	11.12
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG13	10	11.12
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG11	10	11.12
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG12	10	11.12
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG13	10	11.12
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD21	6	11.11
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD22	6	11.11
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD23	6	11.11
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG11	8	11.08
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG12	8	11.08
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG13	8	11.08
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG11	8	11.08
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG12	8	11.08
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG13	8	11.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG11	8	11.08
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG12	8	11.08
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG13	8	11.08
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG21	8	11.07
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG22	8	11.07
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG23	8	11.07
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG21	8	11.07
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG22	8	11.07
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG23	8	11.07
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG21	8	11.07
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG22	8	11.07
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG23	8	11.07
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD21	3	11.04
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD22	3	11.04
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD23	3	11.04
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD21	3	11.04
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD22	3	11.04
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD23	3	11.04
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD21	3	11.04
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD22	3	11.04
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD23	3	11.04
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD21	3	11.04
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD22	3	11.04
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD23	3	11.04
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD21	3	11.04
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD22	3	11.04
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD23	3	11.04
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD21	3	11.04
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD22	3	11.04
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD23	3	11.04
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD11	2	11.04
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD12	2	11.04
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD13	2	11.04
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD11	2	11.04
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD12	2	11.04
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD13	2	11.04
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD11	2	11.04
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD12	2	11.04
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD13	2	11.04
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG21	9	11.04
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG22	9	11.04
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG23	9	11.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG21	9	11.04
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG22	9	11.04
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG23	9	11.04
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG21	9	11.04
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG22	9	11.04
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG23	9	11.04
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB2	1	11.04
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB3	1	11.04
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB2	1	11.04
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB3	1	11.04
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB2	1	11.04
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB3	1	11.04
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD11	4	11.02
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD12	4	11.02
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD13	4	11.02
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD11	4	11.02
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD12	4	11.02
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD13	4	11.02
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD11	4	11.02
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD12	4	11.02
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD13	4	11.02
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD11	1	11.02
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD12	1	11.02
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD13	1	11.02
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG21	1	11.01
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG22	1	11.01
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG23	1	11.01
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG21	1	11.01
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG22	1	11.01
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG23	1	11.01
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD11	3	11.01
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD12	3	11.01
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD13	3	11.01
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD11	3	11.01
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD12	3	11.01
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD13	3	11.01
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD11	3	11.01
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD12	3	11.01
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD13	3	11.01
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	4	11.0
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	4	11.0
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	4	11.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	4	11.0
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	4	11.0
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	4	11.0
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD11	6	11.0
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD12	6	11.0
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD13	6	11.0
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD21	2	10.99
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD22	2	10.99
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD23	2	10.99
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD21	2	10.99
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD22	2	10.99
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD23	2	10.99
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD21	2	10.99
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD22	2	10.99
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD23	2	10.99
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD21	2	10.99
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD22	2	10.99
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD23	2	10.99
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD21	2	10.99
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD22	2	10.99
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD23	2	10.99
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD21	2	10.99
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD22	2	10.99
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD23	2	10.99
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG21	2	10.99
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG22	2	10.99
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG23	2	10.99
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG21	2	10.99
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG22	2	10.99
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG23	2	10.99
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG21	2	10.99
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG22	2	10.99
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG23	2	10.99
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB2	5	10.98
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB3	5	10.98
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB2	5	10.98
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB3	5	10.98
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB2	5	10.98
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB3	5	10.98
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD21	5	10.96
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD22	5	10.96
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD23	5	10.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD21	5	10.96
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD22	5	10.96
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD23	5	10.96
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD21	5	10.96
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD22	5	10.96
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD23	5	10.96
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG21	5	10.95
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG22	5	10.95
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG23	5	10.95
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG21	5	10.95
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG22	5	10.95
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG23	5	10.95
(3,12)	1:518:A:LEU:CG	2:67:C:LEU:H	2	10.94
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD11	5	10.94
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD12	5	10.94
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD13	5	10.94
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD11	7	10.94
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD12	7	10.94
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD13	7	10.94
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD21	9	10.93
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD22	9	10.93
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD23	9	10.93
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD21	9	10.93
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD22	9	10.93
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD23	9	10.93
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD21	9	10.93
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD22	9	10.93
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD23	9	10.93
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG21	4	10.93
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG22	4	10.93
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG23	4	10.93
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG21	4	10.93
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG22	4	10.93
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG23	4	10.93
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD11	1	10.93
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD12	1	10.93
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD13	1	10.93
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD11	1	10.93
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD12	1	10.93
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD13	1	10.93
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD11	1	10.93
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD12	1	10.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD13	1	10.93
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD11	10	10.93
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD12	10	10.93
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD13	10	10.93
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD11	10	10.93
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD12	10	10.93
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD13	10	10.93
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD11	10	10.93
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD12	10	10.93
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD13	10	10.93
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD21	10	10.93
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD22	10	10.93
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD23	10	10.93
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD21	4	10.92
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD22	4	10.92
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD23	4	10.92
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD21	9	10.92
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD22	9	10.92
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD23	9	10.92
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD21	5	10.91
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD22	5	10.91
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD23	5	10.91
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD11	1	10.91
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD12	1	10.91
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD13	1	10.91
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD21	1	10.91
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD22	1	10.91
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD23	1	10.91
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB2	7	10.9
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB3	7	10.9
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB2	7	10.9
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB3	7	10.9
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB2	7	10.9
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB3	7	10.9
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB2	9	10.9
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB3	9	10.9
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB2	9	10.9
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB3	9	10.9
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB2	9	10.9
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB3	9	10.9
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD21	1	10.89
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD22	1	10.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD23	1	10.89
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD21	1	10.89
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD22	1	10.89
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD23	1	10.89
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD21	1	10.89
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD22	1	10.89
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD23	1	10.89
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD21	1	10.89
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD22	1	10.89
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD23	1	10.89
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD21	1	10.89
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD22	1	10.89
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD23	1	10.89
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD21	1	10.89
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD22	1	10.89
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD23	1	10.89
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG21	8	10.87
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG22	8	10.87
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG23	8	10.87
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG21	8	10.87
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG22	8	10.87
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG23	8	10.87
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG21	7	10.85
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG22	7	10.85
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG23	7	10.85
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG21	7	10.85
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG22	7	10.85
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG23	7	10.85
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG21	10	10.85
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG22	10	10.85
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG23	10	10.85
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG21	10	10.85
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG22	10	10.85
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG23	10	10.85
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB2	8	10.85
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB3	8	10.85
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB2	8	10.85
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB3	8	10.85
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB2	8	10.85
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB3	8	10.85
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD11	10	10.84
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD12	10	10.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD13	10	10.84
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD11	5	10.83
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD12	5	10.83
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD13	5	10.83
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD11	5	10.83
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD12	5	10.83
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD13	5	10.83
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD11	5	10.83
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD12	5	10.83
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD13	5	10.83
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD21	2	10.82
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD22	2	10.82
(1,16)	1:544:A:THR:HA	2:8:B:LEU:HD23	2	10.82
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG21	6	10.81
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG22	6	10.81
(1,52)	1:587:A:THR:HG21	2:70:B:VAL:HG23	6	10.81
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG21	6	10.81
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG22	6	10.81
(1,52)	1:587:A:THR:HG22	2:70:B:VAL:HG23	6	10.81
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG21	6	10.81
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG22	6	10.81
(1,52)	1:587:A:THR:HG23	2:70:B:VAL:HG23	6	10.81
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB2	3	10.81
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB3	3	10.81
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB2	3	10.81
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB3	3	10.81
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB2	3	10.81
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB3	3	10.81
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD11	8	10.81
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD12	8	10.81
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD13	8	10.81
(3,12)	1:518:A:LEU:CG	2:67:C:LEU:H	1	10.8
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD11	9	10.8
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD12	9	10.8
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD13	9	10.8
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD11	9	10.8
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD12	9	10.8
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD13	9	10.8
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD11	9	10.8
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD12	9	10.8
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD13	9	10.8
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG11	1	10.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG12	1	10.79
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG13	1	10.79
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG11	1	10.79
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG12	1	10.79
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG13	1	10.79
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG11	1	10.79
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG12	1	10.79
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG13	1	10.79
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG11	4	10.79
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG12	4	10.79
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG13	4	10.79
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG11	4	10.79
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG12	4	10.79
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG13	4	10.79
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG11	4	10.79
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG12	4	10.79
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG13	4	10.79
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG21	3	10.77
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG22	3	10.77
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG23	3	10.77
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG21	3	10.77
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG22	3	10.77
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG23	3	10.77
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD11	8	10.77
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD12	8	10.77
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD13	8	10.77
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD11	8	10.77
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD12	8	10.77
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD13	8	10.77
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB2	10	10.76
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB3	10	10.76
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB2	10	10.76
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB3	10	10.76
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB2	10	10.76
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB3	10	10.76
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD21	4	10.75
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD22	4	10.75
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD23	4	10.75
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD21	4	10.75
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD22	4	10.75
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD23	4	10.75
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD21	4	10.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD22	4	10.75
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD23	4	10.75
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD21	4	10.75
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD22	4	10.75
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD23	4	10.75
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD21	4	10.75
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD22	4	10.75
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD23	4	10.75
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD21	4	10.75
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD22	4	10.75
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD23	4	10.75
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD11	9	10.7
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD12	9	10.7
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD13	9	10.7
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD11	4	10.7
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD12	4	10.7
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD13	4	10.7
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD21	4	10.7
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD22	4	10.7
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD23	4	10.7
(3,12)	1:518:A:LEU:CG	2:67:C:LEU:H	6	10.69
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD11	2	10.69
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD12	2	10.69
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD13	2	10.69
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD11	2	10.69
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD12	2	10.69
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD13	2	10.69
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD11	2	10.69
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD12	2	10.69
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD13	2	10.69
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD11	2	10.69
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD12	2	10.69
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD13	2	10.69
(3,12)	1:518:A:LEU:CG	2:67:C:LEU:H	5	10.67
(3,12)	1:518:A:LEU:CG	2:67:C:LEU:H	10	10.66
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD11	7	10.65
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD12	7	10.65
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD13	7	10.65
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD11	7	10.65
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD12	7	10.65
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD13	7	10.65
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD11	7	10.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD12	7	10.65
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD13	7	10.65
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD11	3	10.65
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD12	3	10.65
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD13	3	10.65
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD11	5	10.64
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD12	5	10.64
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD13	5	10.64
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD11	5	10.64
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD12	5	10.64
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD13	5	10.64
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD11	5	10.64
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD12	5	10.64
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD13	5	10.64
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD11	5	10.64
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD12	5	10.64
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD13	5	10.64
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD11	5	10.64
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD12	5	10.64
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD13	5	10.64
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD11	5	10.64
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD12	5	10.64
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD13	5	10.64
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG21	6	10.63
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG22	6	10.63
(1,59)	1:591:A:ILE:HG21	2:44:B:ILE:HG23	6	10.63
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG21	6	10.63
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG22	6	10.63
(1,59)	1:591:A:ILE:HG22	2:44:B:ILE:HG23	6	10.63
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG21	6	10.63
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG22	6	10.63
(1,59)	1:591:A:ILE:HG23	2:44:B:ILE:HG23	6	10.63
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	6	10.63
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD11	6	10.63
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	6	10.63
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD12	6	10.63
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	6	10.63
(1,30)	1:544:A:THR:HB	2:71:B:LEU:HD13	6	10.63
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD11	2	10.63
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD12	2	10.63
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD13	2	10.63
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD21	2	10.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD22	2	10.63
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD23	2	10.63
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD21	9	10.62
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD22	9	10.62
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD23	9	10.62
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD21	9	10.62
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD22	9	10.62
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD23	9	10.62
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD21	9	10.62
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD22	9	10.62
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD23	9	10.62
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD21	9	10.62
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD22	9	10.62
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD23	9	10.62
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD21	9	10.62
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD22	9	10.62
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD23	9	10.62
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD21	9	10.62
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD22	9	10.62
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD23	9	10.62
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB2	4	10.62
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB3	4	10.62
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB2	4	10.62
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB3	4	10.62
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB2	4	10.62
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB3	4	10.62
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD21	10	10.61
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD22	10	10.61
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD23	10	10.61
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD21	10	10.61
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD22	10	10.61
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD23	10	10.61
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD21	10	10.61
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD22	10	10.61
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD23	10	10.61
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD11	2	10.58
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD12	2	10.58
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD13	2	10.58
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD11	2	10.58
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD12	2	10.58
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD13	2	10.58
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD11	2	10.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD12	2	10.58
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD13	2	10.58
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD11	2	10.58
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD12	2	10.58
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD13	2	10.58
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD11	2	10.58
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD12	2	10.58
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD13	2	10.58
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD11	2	10.58
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD12	2	10.58
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD13	2	10.58
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD11	9	10.57
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD12	9	10.57
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD13	9	10.57
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD11	9	10.57
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD12	9	10.57
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD13	9	10.57
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD11	9	10.57
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD12	9	10.57
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD13	9	10.57
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD21	10	10.56
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD22	10	10.56
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD23	10	10.56
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD21	10	10.56
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD22	10	10.56
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD23	10	10.56
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD21	10	10.56
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD22	10	10.56
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD23	10	10.56
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD21	3	10.55
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD22	3	10.55
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD23	3	10.55
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD21	3	10.55
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD22	3	10.55
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD23	3	10.55
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD11	9	10.54
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD12	9	10.54
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD13	9	10.54
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD21	9	10.54
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD22	9	10.54
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD23	9	10.54
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG21	5	10.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG22	5	10.53
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG23	5	10.53
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG21	5	10.53
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG22	5	10.53
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG23	5	10.53
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG21	5	10.53
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG22	5	10.53
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG23	5	10.53
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD11	9	10.52
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD12	9	10.52
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD13	9	10.52
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD11	9	10.52
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD12	9	10.52
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD13	9	10.52
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD11	9	10.52
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD12	9	10.52
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD13	9	10.52
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD11	3	10.51
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD12	3	10.51
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD13	3	10.51
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD11	3	10.51
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD12	3	10.51
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD13	3	10.51
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD11	3	10.51
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD12	3	10.51
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD13	3	10.51
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD11	7	10.51
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD12	7	10.51
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD13	7	10.51
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD11	7	10.51
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD12	7	10.51
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD13	7	10.51
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD11	7	10.51
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD12	7	10.51
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD13	7	10.51
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG21	9	10.49
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG22	9	10.49
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG23	9	10.49
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG21	9	10.49
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG22	9	10.49
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG23	9	10.49
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD11	6	10.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD12	6	10.48
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD13	6	10.48
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD21	6	10.48
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD22	6	10.48
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD23	6	10.48
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD11	4	10.47
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD12	4	10.47
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD13	4	10.47
(3,12)	1:518:A:LEU:CG	2:67:C:LEU:H	3	10.46
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD21	1	10.46
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD22	1	10.46
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD23	1	10.46
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD21	1	10.46
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD22	1	10.46
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD23	1	10.46
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD21	5	10.46
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD22	5	10.46
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD23	5	10.46
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD21	5	10.46
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD22	5	10.46
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD23	5	10.46
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD21	5	10.46
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD22	5	10.46
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD23	5	10.46
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD21	5	10.46
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD22	5	10.46
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD23	5	10.46
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD21	5	10.46
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD22	5	10.46
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD23	5	10.46
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD21	5	10.46
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD22	5	10.46
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD23	5	10.46
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD11	4	10.46
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD12	4	10.46
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD13	4	10.46
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD11	4	10.46
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD12	4	10.46
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD13	4	10.46
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD11	4	10.46
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD12	4	10.46
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD13	4	10.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:514:A:ALA:HB1	2:73:B:LEU:HG	3	10.46
(1,6)	1:514:A:ALA:HB2	2:73:B:LEU:HG	3	10.46
(1,6)	1:514:A:ALA:HB3	2:73:B:LEU:HG	3	10.46
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD11	5	10.45
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD12	5	10.45
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD13	5	10.45
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD11	8	10.45
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD12	8	10.45
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD13	8	10.45
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD11	8	10.45
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD12	8	10.45
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD13	8	10.45
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD21	7	10.45
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD22	7	10.45
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD23	7	10.45
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD21	7	10.45
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD22	7	10.45
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD23	7	10.45
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD21	7	10.45
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD22	7	10.45
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD23	7	10.45
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD21	7	10.45
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD22	7	10.45
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD23	7	10.45
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD21	7	10.45
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD22	7	10.45
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD23	7	10.45
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD21	7	10.45
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD22	7	10.45
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD23	7	10.45
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD11	3	10.45
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD12	3	10.45
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD13	3	10.45
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD11	3	10.44
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD12	3	10.44
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD13	3	10.44
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD11	1	10.44
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD12	1	10.44
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD13	1	10.44
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD11	1	10.44
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD12	1	10.44
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD13	1	10.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD11	1	10.44
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD12	1	10.44
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD13	1	10.44
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD21	3	10.43
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD22	3	10.43
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD23	3	10.43
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD21	3	10.43
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD22	3	10.43
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD23	3	10.43
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD11	9	10.43
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD12	9	10.43
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD13	9	10.43
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD11	9	10.43
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD12	9	10.43
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD13	9	10.43
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD11	2	10.43
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD12	2	10.43
(1,15)	1:544:A:THR:HA	2:8:B:LEU:HD13	2	10.43
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD21	6	10.42
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD22	6	10.42
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD23	6	10.42
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD21	6	10.42
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD22	6	10.42
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD23	6	10.42
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD21	6	10.42
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD22	6	10.42
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD23	6	10.42
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD21	2	10.42
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD22	2	10.42
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD23	2	10.42
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD21	2	10.42
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD22	2	10.42
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD23	2	10.42
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD11	7	10.4
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD12	7	10.4
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD13	7	10.4
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG21	2	10.38
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG22	2	10.38
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG23	2	10.38
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG21	2	10.38
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG22	2	10.38
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG23	2	10.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG21	2	10.38
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG22	2	10.38
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG23	2	10.38
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD21	4	10.38
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD22	4	10.38
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD23	4	10.38
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD21	4	10.38
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD22	4	10.38
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD23	4	10.38
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD21	4	10.38
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD22	4	10.38
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD23	4	10.38
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD11	7	10.38
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD12	7	10.38
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD13	7	10.38
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD11	7	10.38
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD12	7	10.38
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD13	7	10.38
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD11	7	10.38
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD12	7	10.38
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD13	7	10.38
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD21	5	10.37
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD22	5	10.37
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD23	5	10.37
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD21	5	10.37
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD22	5	10.37
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD23	5	10.37
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD21	5	10.37
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD22	5	10.37
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD23	5	10.37
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD11	1	10.36
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD12	1	10.36
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD13	1	10.36
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD11	1	10.36
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD12	1	10.36
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD13	1	10.36
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD11	1	10.36
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD12	1	10.36
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD13	1	10.36
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD11	6	10.36
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD12	6	10.36
(1,79)	1:511:A:PRO:HB2	2:44:C:ILE:HD13	6	10.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD11	6	10.36
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD12	6	10.36
(1,79)	1:511:A:PRO:HB3	2:44:C:ILE:HD13	6	10.36
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD11	8	10.36
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD12	8	10.36
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD13	8	10.36
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD11	8	10.36
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD12	8	10.36
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD13	8	10.36
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD11	8	10.36
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD12	8	10.36
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD13	8	10.36
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG11	9	10.36
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG12	9	10.36
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG13	9	10.36
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG11	9	10.36
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG12	9	10.36
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG13	9	10.36
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG11	9	10.36
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG12	9	10.36
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG13	9	10.36
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG21	6	10.32
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG22	6	10.32
(1,85)	1:511:A:PRO:HG2	2:70:C:VAL:HG23	6	10.32
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG21	6	10.32
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG22	6	10.32
(1,85)	1:511:A:PRO:HG3	2:70:C:VAL:HG23	6	10.32
(3,12)	1:518:A:LEU:CG	2:67:C:LEU:H	7	10.31
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD21	4	10.31
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD22	4	10.31
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD23	4	10.31
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD21	4	10.31
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD22	4	10.31
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD23	4	10.31
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD11	1	10.31
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD12	1	10.31
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD13	1	10.31
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD11	1	10.31
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD12	1	10.31
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD13	1	10.31
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD11	1	10.31
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD12	1	10.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD13	1	10.31
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD11	1	10.31
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD12	1	10.31
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD13	1	10.31
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD11	1	10.31
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD12	1	10.31
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD13	1	10.31
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD11	1	10.31
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD12	1	10.31
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD13	1	10.31
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD11	5	10.31
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD12	5	10.31
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD13	5	10.31
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD11	5	10.31
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD12	5	10.31
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD13	5	10.31
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG11	2	10.3
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG12	2	10.3
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG13	2	10.3
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG11	2	10.3
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG12	2	10.3
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG13	2	10.3
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG11	2	10.3
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG12	2	10.3
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG13	2	10.3
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD11	3	10.3
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD12	3	10.3
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD13	3	10.3
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD11	3	10.3
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD12	3	10.3
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD13	3	10.3
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD11	3	10.3
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD12	3	10.3
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD13	3	10.3
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD11	5	10.3
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD12	5	10.3
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD13	5	10.3
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD11	5	10.3
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD12	5	10.3
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD13	5	10.3
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD11	5	10.3
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD12	5	10.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD13	5	10.3
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD11	4	10.29
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD12	4	10.29
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD13	4	10.29
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD11	4	10.29
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD12	4	10.29
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD13	4	10.29
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD11	4	10.29
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD12	4	10.29
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD13	4	10.29
(1,64)	1:548:A:ASP:OD2	2:42:B:ARG:NH2	3	10.27
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD21	3	10.26
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD22	3	10.26
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD23	3	10.26
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD21	3	10.26
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD22	3	10.26
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD23	3	10.26
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD21	3	10.26
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD22	3	10.26
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD23	3	10.26
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG11	6	10.25
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG12	6	10.25
(1,51)	1:587:A:THR:HG21	2:70:B:VAL:HG13	6	10.25
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG11	6	10.25
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG12	6	10.25
(1,51)	1:587:A:THR:HG22	2:70:B:VAL:HG13	6	10.25
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG11	6	10.25
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG12	6	10.25
(1,51)	1:587:A:THR:HG23	2:70:B:VAL:HG13	6	10.25
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD11	4	10.25
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD12	4	10.25
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD13	4	10.25
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD11	8	10.24
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD12	8	10.24
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD13	8	10.24
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD11	8	10.24
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD12	8	10.24
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD13	8	10.24
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG21	6	10.24
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG22	6	10.24
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG23	6	10.24
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG21	6	10.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG22	6	10.24
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG23	6	10.24
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG21	6	10.24
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG22	6	10.24
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG23	6	10.24
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD11	3	10.23
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD12	3	10.23
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD13	3	10.23
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD11	3	10.23
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD12	3	10.23
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD13	3	10.23
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD11	3	10.23
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD12	3	10.23
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD13	3	10.23
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD11	3	10.23
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD12	3	10.23
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD13	3	10.23
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD11	3	10.23
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD12	3	10.23
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD13	3	10.23
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD11	3	10.23
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD12	3	10.23
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD13	3	10.23
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD21	2	10.23
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD22	2	10.23
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD23	2	10.23
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD21	2	10.23
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD22	2	10.23
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD23	2	10.23
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD21	2	10.23
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD22	2	10.23
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD23	2	10.23
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD21	8	10.22
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD22	8	10.22
(1,89)	1:512:A:ILE:HD11	2:8:C:LEU:HD23	8	10.22
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD21	8	10.22
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD22	8	10.22
(1,89)	1:512:A:ILE:HD12	2:8:C:LEU:HD23	8	10.22
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD21	8	10.22
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD22	8	10.22
(1,89)	1:512:A:ILE:HD13	2:8:C:LEU:HD23	8	10.22
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD11	7	10.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD12	7	10.22
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD13	7	10.22
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD11	7	10.22
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD12	7	10.22
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD13	7	10.22
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD11	7	10.22
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD12	7	10.22
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD13	7	10.22
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD11	7	10.22
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD12	7	10.22
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD13	7	10.22
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD11	7	10.22
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD12	7	10.22
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD13	7	10.22
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD11	7	10.22
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD12	7	10.22
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD13	7	10.22
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD11	8	10.22
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD12	8	10.22
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD13	8	10.22
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD11	8	10.22
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD12	8	10.22
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD13	8	10.22
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD11	8	10.22
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD12	8	10.22
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD13	8	10.22
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD11	8	10.21
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD12	8	10.21
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD13	8	10.21
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD21	9	10.21
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD22	9	10.21
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD23	9	10.21
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD21	9	10.21
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD22	9	10.21
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD23	9	10.21
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD21	9	10.21
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD22	9	10.21
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD23	9	10.21
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD11	10	10.21
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD12	10	10.21
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD13	10	10.21
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD11	10	10.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD12	10	10.21
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD13	10	10.21
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD11	10	10.21
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD12	10	10.21
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD13	10	10.21
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG21	4	10.2
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG22	4	10.2
(1,60)	1:591:A:ILE:HD11	2:44:B:ILE:HG23	4	10.2
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG21	4	10.2
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG22	4	10.2
(1,60)	1:591:A:ILE:HD12	2:44:B:ILE:HG23	4	10.2
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG21	4	10.2
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG22	4	10.2
(1,60)	1:591:A:ILE:HD13	2:44:B:ILE:HG23	4	10.2
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB2	2	10.2
(1,21)	1:544:A:THR:HG21	2:8:B:LEU:HB3	2	10.2
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB2	2	10.2
(1,21)	1:544:A:THR:HG22	2:8:B:LEU:HB3	2	10.2
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB2	2	10.2
(1,21)	1:544:A:THR:HG23	2:8:B:LEU:HB3	2	10.2
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD11	6	10.19
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD12	6	10.19
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD13	6	10.19
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD11	6	10.19
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD12	6	10.19
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD13	6	10.19
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD11	6	10.19
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD12	6	10.19
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD13	6	10.19
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD21	10	10.19
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD22	10	10.19
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD23	10	10.19
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD21	10	10.19
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD22	10	10.19
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD23	10	10.19
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD21	10	10.19
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD22	10	10.19
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD23	10	10.19
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD21	10	10.19
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD22	10	10.19
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD23	10	10.19
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD21	10	10.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD22	10	10.19
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD23	10	10.19
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD21	10	10.19
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD22	10	10.19
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD23	10	10.19
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD21	8	10.15
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD22	8	10.15
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD23	8	10.15
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD21	8	10.15
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD22	8	10.15
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD23	8	10.15
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD21	8	10.15
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD22	8	10.15
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD23	8	10.15
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD11	4	10.14
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD12	4	10.14
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD13	4	10.14
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD11	4	10.14
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD12	4	10.14
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD13	4	10.14
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD11	4	10.14
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD12	4	10.14
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD13	4	10.14
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD11	4	10.14
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD12	4	10.14
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD13	4	10.14
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD11	4	10.14
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD12	4	10.14
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD13	4	10.14
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD11	4	10.14
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD12	4	10.14
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD13	4	10.14
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD11	6	10.14
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD12	6	10.14
(1,61)	1:591:A:ILE:HG21	2:44:B:ILE:HD13	6	10.14
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD11	6	10.14
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD12	6	10.14
(1,61)	1:591:A:ILE:HG22	2:44:B:ILE:HD13	6	10.14
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD11	6	10.14
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD12	6	10.14
(1,61)	1:591:A:ILE:HG23	2:44:B:ILE:HD13	6	10.14
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD21	3	10.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD22	3	10.1
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD23	3	10.1
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD21	3	10.1
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD22	3	10.1
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD23	3	10.1
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD21	10	10.1
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD22	10	10.1
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD23	10	10.1
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD21	10	10.1
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD22	10	10.1
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD23	10	10.1
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD21	10	10.1
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD22	10	10.1
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD23	10	10.1
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD21	2	10.09
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD22	2	10.09
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD23	2	10.09
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD21	2	10.09
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD22	2	10.09
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD23	2	10.09
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD11	5	10.09
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD12	5	10.09
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD13	5	10.09
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD11	5	10.09
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD12	5	10.09
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD13	5	10.09
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD11	5	10.09
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD12	5	10.09
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD13	5	10.09
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD21	5	10.09
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD22	5	10.09
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD23	5	10.09
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD21	9	10.06
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD22	9	10.06
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD23	9	10.06
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD21	9	10.06
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD22	9	10.06
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD23	9	10.06
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD21	6	10.05
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD22	6	10.05
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD23	6	10.05
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD21	6	10.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD22	6	10.05
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD23	6	10.05
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD21	6	10.05
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD22	6	10.05
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD23	6	10.05
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG21	2	10.04
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG22	2	10.04
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG23	2	10.04
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD11	1	10.03
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD12	1	10.03
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD13	1	10.03
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD21	7	10.03
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD22	7	10.03
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD23	7	10.03
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD21	7	10.03
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD22	7	10.03
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD23	7	10.03
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD21	7	10.03
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD22	7	10.03
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD23	7	10.03
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD21	5	9.99
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD22	5	9.99
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD23	5	9.99
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD21	5	9.99
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD22	5	9.99
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD23	5	9.99
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD21	5	9.99
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD22	5	9.99
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD23	5	9.99
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD21	8	9.97
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD22	8	9.97
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD23	8	9.97
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD11	4	9.96
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD12	4	9.96
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD13	4	9.96
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD21	10	9.95
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD22	10	9.95
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD23	10	9.95
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD21	10	9.95
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD22	10	9.95
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD23	10	9.95
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD11	10	9.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD12	10	9.94
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD13	10	9.94
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD21	5	9.94
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD22	5	9.94
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD23	5	9.94
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD21	5	9.94
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD22	5	9.94
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD23	5	9.94
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD21	1	9.94
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD22	1	9.94
(1,38)	1:547:A:MET:HE1	2:8:B:LEU:HD23	1	9.94
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD21	1	9.94
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD22	1	9.94
(1,38)	1:547:A:MET:HE2	2:8:B:LEU:HD23	1	9.94
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD21	1	9.94
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD22	1	9.94
(1,38)	1:547:A:MET:HE3	2:8:B:LEU:HD23	1	9.94
(3,12)	1:518:A:LEU:CG	2:67:C:LEU:H	9	9.93
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD21	8	9.92
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD22	8	9.92
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD23	8	9.92
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD21	8	9.92
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD22	8	9.92
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD23	8	9.92
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD21	8	9.92
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD22	8	9.92
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD23	8	9.92
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD21	8	9.92
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD22	8	9.92
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD23	8	9.92
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD21	8	9.92
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD22	8	9.92
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD23	8	9.92
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD21	8	9.92
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD22	8	9.92
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD23	8	9.92
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD21	7	9.91
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD22	7	9.91
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD23	7	9.91
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD21	7	9.91
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD22	7	9.91
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD23	7	9.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD21	4	9.91
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD22	4	9.91
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD23	4	9.91
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD21	4	9.91
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD22	4	9.91
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD23	4	9.91
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD21	4	9.91
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD22	4	9.91
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD23	4	9.91
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD21	7	9.91
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD22	7	9.91
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD23	7	9.91
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD21	7	9.91
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD22	7	9.91
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD23	7	9.91
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD21	7	9.91
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD22	7	9.91
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD23	7	9.91
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD21	4	9.88
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD22	4	9.88
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD23	4	9.88
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD21	4	9.88
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD22	4	9.88
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD23	4	9.88
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD11	7	9.88
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD12	7	9.88
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD13	7	9.88
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD21	7	9.88
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD22	7	9.88
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD23	7	9.88
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD21	5	9.87
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD22	5	9.87
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD23	5	9.87
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD21	5	9.87
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD22	5	9.87
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD23	5	9.87
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG21	5	9.87
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG22	5	9.87
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG23	5	9.87
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG21	5	9.87
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG22	5	9.87
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG23	5	9.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG21	5	9.87
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG22	5	9.87
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG23	5	9.87
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD11	5	9.87
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD12	5	9.87
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD13	5	9.87
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD11	5	9.87
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD12	5	9.87
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD13	5	9.87
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD21	8	9.87
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD22	8	9.87
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD23	8	9.87
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD11	9	9.84
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD12	9	9.84
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD13	9	9.84
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD11	9	9.84
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD12	9	9.84
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD13	9	9.84
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD11	9	9.84
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD12	9	9.84
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD13	9	9.84
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD11	9	9.84
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD12	9	9.84
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD13	9	9.84
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD11	9	9.84
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD12	9	9.84
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD13	9	9.84
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD11	9	9.84
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD12	9	9.84
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD13	9	9.84
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD21	3	9.84
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD22	3	9.84
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD23	3	9.84
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD21	1	9.83
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD22	1	9.83
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD23	1	9.83
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD21	1	9.83
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD22	1	9.83
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD23	1	9.83
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD11	9	9.82
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD12	9	9.82
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD13	9	9.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD11	9	9.82
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD12	9	9.82
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD13	9	9.82
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD11	9	9.82
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD12	9	9.82
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD13	9	9.82
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD21	6	9.82
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD22	6	9.82
(1,77)	1:508:A:LEU:HD11	2:8:C:LEU:HD23	6	9.82
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD21	6	9.82
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD22	6	9.82
(1,77)	1:508:A:LEU:HD12	2:8:C:LEU:HD23	6	9.82
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD21	6	9.82
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD22	6	9.82
(1,77)	1:508:A:LEU:HD13	2:8:C:LEU:HD23	6	9.82
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD21	6	9.82
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD22	6	9.82
(1,77)	1:508:A:LEU:HD21	2:8:C:LEU:HD23	6	9.82
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD21	6	9.82
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD22	6	9.82
(1,77)	1:508:A:LEU:HD22	2:8:C:LEU:HD23	6	9.82
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD21	6	9.82
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD22	6	9.82
(1,77)	1:508:A:LEU:HD23	2:8:C:LEU:HD23	6	9.82
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD21	3	9.82
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD22	3	9.82
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD23	3	9.82
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD21	3	9.82
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD22	3	9.82
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD23	3	9.82
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD21	3	9.82
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD22	3	9.82
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD23	3	9.82
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD21	6	9.82
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD22	6	9.82
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD23	6	9.82
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD21	6	9.82
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD22	6	9.82
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD23	6	9.82
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD21	6	9.82
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD22	6	9.82
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD23	6	9.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD21	9	9.81
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD22	9	9.81
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD23	9	9.81
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD21	9	9.81
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD22	9	9.81
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD23	9	9.81
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD21	9	9.81
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD22	9	9.81
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD23	9	9.81
(3,12)	1:518:A:LEU:CG	2:67:C:LEU:H	4	9.8
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD11	9	9.79
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD12	9	9.79
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD13	9	9.79
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD11	9	9.79
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD12	9	9.79
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD13	9	9.79
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD11	9	9.79
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD12	9	9.79
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD13	9	9.79
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD11	7	9.78
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD12	7	9.78
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD13	7	9.78
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD11	7	9.78
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD12	7	9.78
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD13	7	9.78
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD11	7	9.78
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD12	7	9.78
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD13	7	9.78
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD11	1	9.77
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD12	1	9.77
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD13	1	9.77
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD11	1	9.77
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD12	1	9.77
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD13	1	9.77
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD11	1	9.77
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD12	1	9.77
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD13	1	9.77
(3,1)	1:518:A:LEU:CG	2:6:C:LYS:H	8	9.76
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD11	10	9.73
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD12	10	9.73
(1,88)	1:512:A:ILE:HD11	2:8:C:LEU:HD13	10	9.73
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD11	10	9.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD12	10	9.73
(1,88)	1:512:A:ILE:HD12	2:8:C:LEU:HD13	10	9.73
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD11	10	9.73
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD12	10	9.73
(1,88)	1:512:A:ILE:HD13	2:8:C:LEU:HD13	10	9.73
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG21	6	9.72
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG22	6	9.72
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG23	6	9.72
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG21	6	9.72
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG22	6	9.72
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG23	6	9.72
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG21	6	9.72
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG22	6	9.72
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG23	6	9.72
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD21	7	9.71
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD22	7	9.71
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD23	7	9.71
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD11	6	9.7
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD12	6	9.7
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD13	6	9.7
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD21	1	9.69
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD22	1	9.69
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD23	1	9.69
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG21	3	9.68
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG22	3	9.68
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG23	3	9.68
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG21	3	9.68
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG22	3	9.68
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG23	3	9.68
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG21	3	9.68
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG22	3	9.68
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG23	3	9.68
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD11	6	9.68
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD12	6	9.68
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD13	6	9.68
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD11	6	9.68
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD12	6	9.68
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD13	6	9.68
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD11	6	9.68
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD12	6	9.68
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD13	6	9.68
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD11	6	9.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD12	6	9.68
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD13	6	9.68
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD11	6	9.68
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD12	6	9.68
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD13	6	9.68
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD11	6	9.68
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD12	6	9.68
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD13	6	9.68
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD21	8	9.68
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD22	8	9.68
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD23	8	9.68
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD21	8	9.68
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD22	8	9.68
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD23	8	9.68
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD21	8	9.68
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD22	8	9.68
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD23	8	9.68
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG21	1	9.66
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG22	1	9.66
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG23	1	9.66
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG21	1	9.66
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG22	1	9.66
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG23	1	9.66
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG21	1	9.66
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG22	1	9.66
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG23	1	9.66
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD11	2	9.66
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD12	2	9.66
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD13	2	9.66
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD11	2	9.66
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD12	2	9.66
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD13	2	9.66
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD11	4	9.66
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD12	4	9.66
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD13	4	9.66
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD11	4	9.66
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD12	4	9.66
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD13	4	9.66
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD11	4	9.66
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD12	4	9.66
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD13	4	9.66
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD11	10	9.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD12	10	9.65
(1,76)	1:508:A:LEU:HD11	2:8:C:LEU:HD13	10	9.65
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD11	10	9.65
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD12	10	9.65
(1,76)	1:508:A:LEU:HD12	2:8:C:LEU:HD13	10	9.65
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD11	10	9.65
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD12	10	9.65
(1,76)	1:508:A:LEU:HD13	2:8:C:LEU:HD13	10	9.65
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD11	10	9.65
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD12	10	9.65
(1,76)	1:508:A:LEU:HD21	2:8:C:LEU:HD13	10	9.65
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD11	10	9.65
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD12	10	9.65
(1,76)	1:508:A:LEU:HD22	2:8:C:LEU:HD13	10	9.65
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD11	10	9.65
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD12	10	9.65
(1,76)	1:508:A:LEU:HD23	2:8:C:LEU:HD13	10	9.65
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD21	2	9.65
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD22	2	9.65
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD23	2	9.65
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD21	2	9.65
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD22	2	9.65
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD23	2	9.65
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD21	2	9.65
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD22	2	9.65
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD23	2	9.65
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG21	7	9.64
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG22	7	9.64
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG23	7	9.64
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG21	7	9.64
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG22	7	9.64
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG23	7	9.64
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG21	7	9.64
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG22	7	9.64
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG23	7	9.64
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD11	5	9.64
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD12	5	9.64
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD13	5	9.64
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD11	5	9.64
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD12	5	9.64
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD13	5	9.64
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD11	5	9.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD12	5	9.64
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD13	5	9.64
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG21	5	9.62
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG22	5	9.62
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG23	5	9.62
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG21	2	9.62
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG22	2	9.62
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG23	2	9.62
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG21	2	9.62
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG22	2	9.62
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG23	2	9.62
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG21	2	9.62
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG22	2	9.62
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG23	2	9.62
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG21	4	9.62
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG22	4	9.62
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG23	4	9.62
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG21	4	9.62
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG22	4	9.62
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG23	4	9.62
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG21	4	9.62
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG22	4	9.62
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG23	4	9.62
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD21	5	9.62
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD22	5	9.62
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD23	5	9.62
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD21	5	9.62
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD22	5	9.62
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD23	5	9.62
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD21	5	9.62
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD22	5	9.62
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD23	5	9.62
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD11	6	9.61
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD12	6	9.61
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD13	6	9.61
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD11	6	9.61
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD12	6	9.61
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD13	6	9.61
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD11	6	9.61
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD12	6	9.61
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD13	6	9.61
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD21	1	9.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD22	1	9.61
(1,14)	1:543:A:THR:HG21	2:8:B:LEU:HD23	1	9.61
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD21	1	9.61
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD22	1	9.61
(1,14)	1:543:A:THR:HG22	2:8:B:LEU:HD23	1	9.61
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD21	1	9.61
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD22	1	9.61
(1,14)	1:543:A:THR:HG23	2:8:B:LEU:HD23	1	9.61
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD11	4	9.61
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD12	4	9.61
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD13	4	9.61
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD11	4	9.61
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD12	4	9.61
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD13	4	9.61
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD11	4	9.61
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD12	4	9.61
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD13	4	9.61
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD21	6	9.6
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD22	6	9.6
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD23	6	9.6
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD21	6	9.6
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD22	6	9.6
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD23	6	9.6
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD21	1	9.6
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD22	1	9.6
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD23	1	9.6
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD11	6	9.59
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD12	6	9.59
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD13	6	9.59
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD11	6	9.59
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD12	6	9.59
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD13	6	9.59
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD11	6	9.59
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD12	6	9.59
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD13	6	9.59
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD21	7	9.58
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD22	7	9.58
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD23	7	9.58
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD21	7	9.58
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD22	7	9.58
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD23	7	9.58
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG21	4	9.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG22	4	9.56
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG23	4	9.56
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG21	4	9.56
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG22	4	9.56
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG23	4	9.56
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG21	4	9.56
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG22	4	9.56
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG23	4	9.56
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG21	4	9.56
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG22	4	9.56
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG23	4	9.56
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG21	4	9.56
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG22	4	9.56
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG23	4	9.56
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG21	4	9.56
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG22	4	9.56
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG23	4	9.56
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD11	10	9.54
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD12	10	9.54
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD13	10	9.54
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD11	10	9.54
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD12	10	9.54
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD13	10	9.54
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD11	10	9.54
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD12	10	9.54
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD13	10	9.54
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG21	8	9.53
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG22	8	9.53
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG23	8	9.53
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD21	4	9.53
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD22	4	9.53
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD23	4	9.53
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD11	2	9.52
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD12	2	9.52
(1,62)	1:591:A:ILE:HD11	2:44:B:ILE:HD13	2	9.52
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD11	2	9.52
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD12	2	9.52
(1,62)	1:591:A:ILE:HD12	2:44:B:ILE:HD13	2	9.52
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD11	2	9.52
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD12	2	9.52
(1,62)	1:591:A:ILE:HD13	2:44:B:ILE:HD13	2	9.52
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG21	2	9.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG22	2	9.51
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG23	2	9.51
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD11	1	9.51
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD12	1	9.51
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD13	1	9.51
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD11	1	9.51
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD12	1	9.51
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD13	1	9.51
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD11	2	9.51
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD12	2	9.51
(1,37)	1:547:A:MET:HE1	2:8:B:LEU:HD13	2	9.51
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD11	2	9.51
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD12	2	9.51
(1,37)	1:547:A:MET:HE2	2:8:B:LEU:HD13	2	9.51
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD11	2	9.51
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD12	2	9.51
(1,37)	1:547:A:MET:HE3	2:8:B:LEU:HD13	2	9.51
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD21	6	9.51
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD22	6	9.51
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD23	6	9.51
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD21	3	9.5
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD22	3	9.5
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD23	3	9.5
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD21	3	9.5
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD22	3	9.5
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD23	3	9.5
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD21	3	9.5
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD22	3	9.5
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD23	3	9.5
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG21	7	9.49
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG22	7	9.49
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG23	7	9.49
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG21	8	9.48
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG22	8	9.48
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG23	8	9.48
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG21	8	9.48
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG22	8	9.48
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG23	8	9.48
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG21	8	9.48
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG22	8	9.48
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG23	8	9.48
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG21	6	9.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG22	6	9.47
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG23	6	9.47
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG21	6	9.47
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG22	6	9.47
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG23	6	9.47
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG21	6	9.47
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG22	6	9.47
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG23	6	9.47
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG21	6	9.47
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG22	6	9.47
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG23	6	9.47
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG21	6	9.47
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG22	6	9.47
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG23	6	9.47
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG21	6	9.47
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG22	6	9.47
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG23	6	9.47
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD21	9	9.45
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD22	9	9.45
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD23	9	9.45
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD21	9	9.45
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD22	9	9.45
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD23	9	9.45
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG21	9	9.45
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG22	9	9.45
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG23	9	9.45
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG21	9	9.45
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG22	9	9.45
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG23	9	9.45
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG21	9	9.45
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG22	9	9.45
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG23	9	9.45
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD21	8	9.44
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD22	8	9.44
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD23	8	9.44
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD21	8	9.44
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD22	8	9.44
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD23	8	9.44
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD21	8	9.44
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD22	8	9.44
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD23	8	9.44
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD11	8	9.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD12	8	9.44
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD13	8	9.44
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD11	8	9.44
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD12	8	9.44
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD13	8	9.44
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD11	8	9.44
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD12	8	9.44
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD13	8	9.44
(1,65)	1:552:A:GLU:OE1	2:42:B:ARG:NH1	4	9.42
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD21	9	9.42
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD22	9	9.42
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD23	9	9.42
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD21	10	9.42
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD22	10	9.42
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD23	10	9.42
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD11	3	9.42
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD12	3	9.42
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD13	3	9.42
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD11	3	9.42
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD12	3	9.42
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD13	3	9.42
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD11	3	9.42
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD12	3	9.42
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD13	3	9.42
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG21	5	9.41
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG22	5	9.41
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG23	5	9.41
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG21	5	9.41
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG22	5	9.41
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG23	5	9.41
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG21	5	9.41
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG22	5	9.41
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG23	5	9.41
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG21	5	9.41
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG22	5	9.41
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG23	5	9.41
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG21	5	9.41
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG22	5	9.41
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG23	5	9.41
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG21	5	9.41
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG22	5	9.41
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG23	5	9.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG21	1	9.39
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG22	1	9.39
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG23	1	9.39
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG21	1	9.39
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG22	1	9.39
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG23	1	9.39
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG21	1	9.39
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG22	1	9.39
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG23	1	9.39
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG21	1	9.39
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG22	1	9.39
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG23	1	9.39
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG21	1	9.39
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG22	1	9.39
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG23	1	9.39
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG21	1	9.39
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG22	1	9.39
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG23	1	9.39
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG21	3	9.38
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG22	3	9.38
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG23	3	9.38
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD21	6	9.37
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD22	6	9.37
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD23	6	9.37
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD21	6	9.37
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD22	6	9.37
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD23	6	9.37
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD11	4	9.37
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD12	4	9.37
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD13	4	9.37
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD11	4	9.37
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD12	4	9.37
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD13	4	9.37
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG21	2	9.37
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG22	2	9.37
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG23	2	9.37
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG21	2	9.37
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG22	2	9.37
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG23	2	9.37
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG21	2	9.37
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG22	2	9.37
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG23	2	9.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG21	2	9.37
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG22	2	9.37
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG23	2	9.37
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG21	2	9.37
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG22	2	9.37
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG23	2	9.37
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG21	2	9.37
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG22	2	9.37
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG23	2	9.37
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG11	7	9.37
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG12	7	9.37
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG13	7	9.37
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD11	7	9.36
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD12	7	9.36
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD13	7	9.36
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD11	7	9.36
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD12	7	9.36
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD13	7	9.36
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD21	5	9.35
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD22	5	9.35
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD23	5	9.35
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD21	5	9.35
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD22	5	9.35
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD23	5	9.35
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD21	1	9.35
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD22	1	9.35
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD23	1	9.35
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD21	1	9.35
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD22	1	9.35
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD23	1	9.35
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD21	1	9.35
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD22	1	9.35
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD23	1	9.35
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG21	1	9.34
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG22	1	9.34
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG23	1	9.34
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD21	7	9.34
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD22	7	9.34
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD23	7	9.34
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD21	7	9.34
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD22	7	9.34
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD23	7	9.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD21	7	9.34
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD22	7	9.34
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD23	7	9.34
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD11	2	9.33
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD12	2	9.33
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD13	2	9.33
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD21	2	9.33
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD22	2	9.33
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD23	2	9.33
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD11	2	9.33
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD12	2	9.33
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD13	2	9.33
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD11	2	9.33
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD12	2	9.33
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD13	2	9.33
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD11	2	9.33
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD12	2	9.33
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD13	2	9.33
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG21	5	9.32
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG22	5	9.32
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG23	5	9.32
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG11	5	9.32
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG12	5	9.32
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG13	5	9.32
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD11	6	9.31
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD12	6	9.31
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD13	6	9.31
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG21	10	9.3
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG22	10	9.3
(1,90)	1:512:A:ILE:HD11	2:9:C:THR:HG23	10	9.3
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG21	10	9.3
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG22	10	9.3
(1,90)	1:512:A:ILE:HD12	2:9:C:THR:HG23	10	9.3
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG21	10	9.3
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG22	10	9.3
(1,90)	1:512:A:ILE:HD13	2:9:C:THR:HG23	10	9.3
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD11	5	9.3
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD12	5	9.3
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD13	5	9.3
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD21	5	9.3
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD22	5	9.3
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD23	5	9.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD11	6	9.29
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD12	6	9.29
(1,13)	1:543:A:THR:HG21	2:8:B:LEU:HD13	6	9.29
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD11	6	9.29
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD12	6	9.29
(1,13)	1:543:A:THR:HG22	2:8:B:LEU:HD13	6	9.29
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD11	6	9.29
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD12	6	9.29
(1,13)	1:543:A:THR:HG23	2:8:B:LEU:HD13	6	9.29
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD11	6	9.28
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD12	6	9.28
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD13	6	9.28
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD11	6	9.28
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD12	6	9.28
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD13	6	9.28
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD11	6	9.28
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD12	6	9.28
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD13	6	9.28
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD11	1	9.28
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD12	1	9.28
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD13	1	9.28
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD21	10	9.27
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD22	10	9.27
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD23	10	9.27
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD21	10	9.27
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD22	10	9.27
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD23	10	9.27
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG21	4	9.27
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG22	4	9.27
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG23	4	9.27
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG21	3	9.27
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG22	3	9.27
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG23	3	9.27
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG21	3	9.27
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG22	3	9.27
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG23	3	9.27
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG21	3	9.27
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG22	3	9.27
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG23	3	9.27
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG21	3	9.27
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG22	3	9.27
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG23	3	9.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG21	3	9.27
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG22	3	9.27
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG23	3	9.27
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG21	3	9.27
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG22	3	9.27
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG23	3	9.27
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD21	9	9.27
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD22	9	9.27
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD23	9	9.27
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD21	9	9.27
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD22	9	9.27
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD23	9	9.27
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD21	9	9.27
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD22	9	9.27
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD23	9	9.27
(1,65)	1:552:A:GLU:OE1	2:42:B:ARG:NH1	7	9.26
(3,1)	1:518:A:LEU:CG	2:6:C:LYS:H	3	9.25
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG21	4	9.25
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG22	4	9.25
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG23	4	9.25
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG21	1	9.25
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG22	1	9.25
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG23	1	9.25
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG21	5	9.25
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG22	5	9.25
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG23	5	9.25
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD11	3	9.25
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD12	3	9.25
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD13	3	9.25
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD11	3	9.25
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD12	3	9.25
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD13	3	9.25
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG11	3	9.25
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG12	3	9.25
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG13	3	9.25
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD11	6	9.24
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD12	6	9.24
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD13	6	9.24
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD11	6	9.24
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD12	6	9.24
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD13	6	9.24
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD21	6	9.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD22	6	9.24
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD23	6	9.24
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD21	6	9.24
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD22	6	9.24
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD23	6	9.24
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD21	6	9.24
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD22	6	9.24
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD23	6	9.24
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG21	10	9.23
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG22	10	9.23
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG23	10	9.23
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD11	1	9.23
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD12	1	9.23
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD13	1	9.23
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD11	1	9.23
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD12	1	9.23
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD13	1	9.23
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD11	1	9.23
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD12	1	9.23
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD13	1	9.23
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG21	7	9.23
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG22	7	9.23
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG23	7	9.23
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD21	4	9.23
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD22	4	9.23
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD23	4	9.23
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD21	4	9.23
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD22	4	9.23
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD23	4	9.23
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD21	4	9.23
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD22	4	9.23
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD23	4	9.23
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD11	5	9.23
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD12	5	9.23
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD13	5	9.23
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG21	1	9.21
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG22	1	9.21
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG23	1	9.21
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD21	2	9.19
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD22	2	9.19
(1,18)	1:544:A:THR:HB	2:8:B:LEU:HD23	2	9.19
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD11	3	9.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD12	3	9.18
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD13	3	9.18
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD11	3	9.18
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD12	3	9.18
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD13	3	9.18
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG21	3	9.18
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG22	3	9.18
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG23	3	9.18
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG21	8	9.17
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG22	8	9.17
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG23	8	9.17
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG21	9	9.16
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG22	9	9.16
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG23	9	9.16
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG21	9	9.16
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG22	9	9.16
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG23	9	9.16
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG21	9	9.16
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG22	9	9.16
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG23	9	9.16
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG21	9	9.16
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG22	9	9.16
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG23	9	9.16
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG21	9	9.16
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG22	9	9.16
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG23	9	9.16
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG21	9	9.16
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG22	9	9.16
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG23	9	9.16
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD11	7	9.16
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD12	7	9.16
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD13	7	9.16
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD11	8	9.15
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD12	8	9.15
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD13	8	9.15
(3,1)	1:518:A:LEU:CG	2:6:C:LYS:H	2	9.14
(3,1)	1:518:A:LEU:CG	2:6:C:LYS:H	1	9.12
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG21	7	9.12
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG22	7	9.12
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG23	7	9.12
(1,64)	1:548:A:ASP:OD2	2:42:B:ARG:NH2	6	9.12
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD11	6	9.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD12	6	9.12
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD13	6	9.12
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD11	4	9.11
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD12	4	9.11
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD13	4	9.11
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD11	4	9.11
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD12	4	9.11
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD13	4	9.11
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG21	10	9.11
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG22	10	9.11
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG23	10	9.11
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD11	5	9.09
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD12	5	9.09
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD13	5	9.09
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD11	5	9.09
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD12	5	9.09
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD13	5	9.09
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD11	4	9.09
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD12	4	9.09
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD13	4	9.09
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD11	4	9.09
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD12	4	9.09
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD13	4	9.09
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD11	4	9.09
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD12	4	9.09
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD13	4	9.09
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG21	8	9.09
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG22	8	9.09
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG23	8	9.09
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD21	10	9.09
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD22	10	9.09
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD23	10	9.09
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD21	10	9.09
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD22	10	9.09
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD23	10	9.09
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD21	10	9.09
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD22	10	9.09
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD23	10	9.09
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG21	10	9.06
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG22	10	9.06
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG23	10	9.06
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD11	9	9.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD12	9	9.05
(1,91)	1:515:A:SER:HA	2:44:C:ILE:HD13	9	9.05
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG21	10	9.05
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG22	10	9.05
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG23	10	9.05
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG21	10	9.05
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG22	10	9.05
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG23	10	9.05
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG21	10	9.05
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG22	10	9.05
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG23	10	9.05
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG21	10	9.05
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG22	10	9.05
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG23	10	9.05
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG21	10	9.05
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG22	10	9.05
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG23	10	9.05
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG21	10	9.05
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG22	10	9.05
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG23	10	9.05
(1,6)	1:514:A:ALA:HB1	2:73:B:LEU:HG	5	9.05
(1,6)	1:514:A:ALA:HB2	2:73:B:LEU:HG	5	9.05
(1,6)	1:514:A:ALA:HB3	2:73:B:LEU:HG	5	9.05
(3,10)	1:518:A:LEU:CG	2:51:C:GLU:H	8	9.04
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD11	1	9.04
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD12	1	9.04
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD13	1	9.04
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD21	1	9.04
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD22	1	9.04
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD23	1	9.04
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD11	10	9.04
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD12	10	9.04
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD13	10	9.04
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG11	8	9.02
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG12	8	9.02
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG13	8	9.02
(3,1)	1:518:A:LEU:CG	2:6:C:LYS:H	6	9.01
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG21	3	9.01
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG22	3	9.01
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG23	3	9.01
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD11	2	9.01
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD12	2	9.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD13	2	9.01
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD11	3	9.01
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD12	3	9.01
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD13	3	9.01
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD11	10	8.99
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD12	10	8.99
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD13	10	8.99
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD11	10	8.99
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD12	10	8.99
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD13	10	8.99
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG21	9	8.99
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG22	9	8.99
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG23	9	8.99
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG21	6	8.98
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG22	6	8.98
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG23	6	8.98
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG21	4	8.98
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG22	4	8.98
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG23	4	8.98
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG21	7	8.97
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG22	7	8.97
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG23	7	8.97
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG21	7	8.97
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG22	7	8.97
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG23	7	8.97
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG21	7	8.97
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG22	7	8.97
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG23	7	8.97
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG21	7	8.97
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG22	7	8.97
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG23	7	8.97
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG21	7	8.97
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG22	7	8.97
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG23	7	8.97
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG21	7	8.97
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG22	7	8.97
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG23	7	8.97
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG21	8	8.96
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG22	8	8.96
(1,75)	1:508:A:LEU:HD11	2:9:C:THR:HG23	8	8.96
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG21	8	8.96
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG22	8	8.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:508:A:LEU:HD12	2:9:C:THR:HG23	8	8.96
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG21	8	8.96
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG22	8	8.96
(1,75)	1:508:A:LEU:HD13	2:9:C:THR:HG23	8	8.96
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG21	8	8.96
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG22	8	8.96
(1,75)	1:508:A:LEU:HD21	2:9:C:THR:HG23	8	8.96
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG21	8	8.96
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG22	8	8.96
(1,75)	1:508:A:LEU:HD22	2:9:C:THR:HG23	8	8.96
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG21	8	8.96
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG22	8	8.96
(1,75)	1:508:A:LEU:HD23	2:9:C:THR:HG23	8	8.96
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD11	1	8.96
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD12	1	8.96
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD13	1	8.96
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD11	1	8.96
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD12	1	8.96
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD13	1	8.96
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD11	1	8.96
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD12	1	8.96
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD13	1	8.96
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD11	3	8.95
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD12	3	8.95
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD13	3	8.95
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD21	3	8.95
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD22	3	8.95
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD23	3	8.95
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG11	4	8.95
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG12	4	8.95
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG13	4	8.95
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD11	9	8.93
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD12	9	8.93
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD13	9	8.93
(1,64)	1:548:A:ASP:OD2	2:42:B:ARG:NH2	8	8.92
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG11	10	8.91
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG12	10	8.91
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG13	10	8.91
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD11	6	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD12	6	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD13	6	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD21	6	8.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD22	6	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD23	6	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD11	8	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD12	8	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD13	8	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD21	8	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD22	8	8.9
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD23	8	8.9
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD11	9	8.9
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD12	9	8.9
(1,80)	1:511:A:PRO:HG2	2:8:C:LEU:HD13	9	8.9
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD11	9	8.9
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD12	9	8.9
(1,80)	1:511:A:PRO:HG3	2:8:C:LEU:HD13	9	8.9
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG11	2	8.88
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG12	2	8.88
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG13	2	8.88
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG11	2	8.88
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG12	2	8.88
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG13	2	8.88
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD11	9	8.88
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD12	9	8.88
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD13	9	8.88
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD11	9	8.88
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD12	9	8.88
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD13	9	8.88
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD11	9	8.88
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD12	9	8.88
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD13	9	8.88
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD21	2	8.88
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD22	2	8.88
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD23	2	8.88
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG11	1	8.86
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG12	1	8.86
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG13	1	8.86
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD11	4	8.86
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD12	4	8.86
(1,17)	1:544:A:THR:HB	2:8:B:LEU:HD13	4	8.86
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD11	4	8.84
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD12	4	8.84
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD13	4	8.84
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD21	4	8.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD22	4	8.84
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD23	4	8.84
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD11	3	8.83
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD12	3	8.83
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD13	3	8.83
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD11	3	8.83
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD12	3	8.83
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD13	3	8.83
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD11	3	8.83
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD12	3	8.83
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD13	3	8.83
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD11	5	8.82
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD12	5	8.82
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD13	5	8.82
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD11	5	8.82
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD12	5	8.82
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD13	5	8.82
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD11	5	8.82
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD12	5	8.82
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD13	5	8.82
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD21	2	8.8
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD22	2	8.8
(1,23)	1:544:A:THR:HG21	2:8:B:LEU:HD23	2	8.8
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD21	2	8.8
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD22	2	8.8
(1,23)	1:544:A:THR:HG22	2:8:B:LEU:HD23	2	8.8
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD21	2	8.8
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD22	2	8.8
(1,23)	1:544:A:THR:HG23	2:8:B:LEU:HD23	2	8.8
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD11	2	8.79
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD12	2	8.79
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD13	2	8.79
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD11	9	8.79
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD12	9	8.79
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD13	9	8.79
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD11	9	8.79
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD12	9	8.79
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD13	9	8.79
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD11	9	8.79
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD12	9	8.79
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD13	9	8.79
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD11	2	8.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD12	2	8.78
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD13	2	8.78
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD11	2	8.78
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD12	2	8.78
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD13	2	8.78
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD11	2	8.78
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD12	2	8.78
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD13	2	8.78
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD11	7	8.77
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD12	7	8.77
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD13	7	8.77
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD11	7	8.77
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD12	7	8.77
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD13	7	8.77
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD11	7	8.77
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD12	7	8.77
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD13	7	8.77
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD11	7	8.76
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD12	7	8.76
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD13	7	8.76
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD21	7	8.76
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD22	7	8.76
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD23	7	8.76
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD11	8	8.76
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD12	8	8.76
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD13	8	8.76
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD11	8	8.76
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD12	8	8.76
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD13	8	8.76
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD11	8	8.76
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD12	8	8.76
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD13	8	8.76
(1,6)	1:514:A:ALA:HB1	2:73:B:LEU:HG	2	8.76
(1,6)	1:514:A:ALA:HB2	2:73:B:LEU:HG	2	8.76
(1,6)	1:514:A:ALA:HB3	2:73:B:LEU:HG	2	8.76
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG11	1	8.75
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG12	1	8.75
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG13	1	8.75
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG11	1	8.75
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG12	1	8.75
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG13	1	8.75
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD11	10	8.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD12	10	8.75
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD13	10	8.75
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD21	10	8.75
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD22	10	8.75
(1,8)	1:541:A:ASP:HA	2:73:B:LEU:HD23	10	8.75
(1,6)	1:514:A:ALA:HB1	2:73:B:LEU:HG	8	8.75
(1,6)	1:514:A:ALA:HB2	2:73:B:LEU:HG	8	8.75
(1,6)	1:514:A:ALA:HB3	2:73:B:LEU:HG	8	8.75
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG11	8	8.74
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG12	8	8.74
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG13	8	8.74
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG11	8	8.74
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG12	8	8.74
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG13	8	8.74
(3,1)	1:518:A:LEU:CG	2:6:C:LYS:H	5	8.73
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD21	8	8.73
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD22	8	8.73
(1,81)	1:511:A:PRO:HG2	2:8:C:LEU:HD23	8	8.73
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD21	8	8.73
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD22	8	8.73
(1,81)	1:511:A:PRO:HG3	2:8:C:LEU:HD23	8	8.73
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD21	9	8.72
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD22	9	8.72
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD23	9	8.72
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD11	1	8.72
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD12	1	8.72
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD13	1	8.72
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD11	2	8.71
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD12	2	8.71
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD13	2	8.71
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD11	2	8.71
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD12	2	8.71
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD13	2	8.71
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD11	3	8.71
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD12	3	8.71
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD13	3	8.71
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD11	3	8.71
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD12	3	8.71
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD13	3	8.71
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD11	3	8.71
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD12	3	8.71
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD13	3	8.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD11	10	8.71
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD12	10	8.71
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD13	10	8.71
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD11	10	8.71
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD12	10	8.71
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD13	10	8.71
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD11	10	8.71
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD12	10	8.71
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD13	10	8.71
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG11	5	8.7
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG12	5	8.7
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG13	5	8.7
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG11	5	8.7
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG12	5	8.7
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG13	5	8.7
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG21	2	8.67
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG22	2	8.67
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG23	2	8.67
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG21	2	8.67
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG22	2	8.67
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG23	2	8.67
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG21	6	8.67
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG22	6	8.67
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG23	6	8.67
(1,64)	1:548:A:ASP:OD2	2:42:B:ARG:NH2	7	8.66
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD11	2	8.66
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD12	2	8.66
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD13	2	8.66
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD11	2	8.66
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD12	2	8.66
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD13	2	8.66
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD11	2	8.66
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD12	2	8.66
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD13	2	8.66
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG21	2	8.66
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG22	2	8.66
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG23	2	8.66
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD21	3	8.66
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD22	3	8.66
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD23	3	8.66
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG11	4	8.65
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG12	4	8.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG13	4	8.65
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG11	4	8.65
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG12	4	8.65
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG13	4	8.65
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD21	8	8.64
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD22	8	8.64
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD23	8	8.64
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD21	8	8.64
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD22	8	8.64
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD23	8	8.64
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG11	3	8.63
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG12	3	8.63
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG13	3	8.63
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG11	3	8.63
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG12	3	8.63
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG13	3	8.63
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG11	3	8.63
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG12	3	8.63
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG13	3	8.63
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG21	6	8.63
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG22	6	8.63
(1,25)	1:544:A:THR:HA	2:70:B:VAL:HG23	6	8.63
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG21	9	8.61
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG22	9	8.61
(1,94)	1:515:A:SER:HA	2:70:C:VAL:HG23	9	8.61
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG11	7	8.61
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG12	7	8.61
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG13	7	8.61
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG11	7	8.61
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG12	7	8.61
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG13	7	8.61
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG21	9	8.61
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG22	9	8.61
(1,83)	1:511:A:PRO:HA	2:70:C:VAL:HG23	9	8.61
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD21	4	8.59
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD22	4	8.59
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD23	4	8.59
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD21	6	8.59
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD22	6	8.59
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD23	6	8.59
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG11	7	8.59
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG12	7	8.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG13	7	8.59
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG11	10	8.58
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG12	10	8.58
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG13	10	8.58
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG11	10	8.58
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG12	10	8.58
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG13	10	8.58
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG11	7	8.58
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG12	7	8.58
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG13	7	8.58
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG11	7	8.58
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG12	7	8.58
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG13	7	8.58
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG11	7	8.58
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG12	7	8.58
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG13	7	8.58
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG11	5	8.57
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG12	5	8.57
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG13	5	8.57
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG21	8	8.56
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG22	8	8.56
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG23	8	8.56
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG21	8	8.56
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG22	8	8.56
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG23	8	8.56
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG11	5	8.56
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG12	5	8.56
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG13	5	8.56
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG11	5	8.56
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG12	5	8.56
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG13	5	8.56
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG11	5	8.56
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG12	5	8.56
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG13	5	8.56
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG11	3	8.56
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG12	3	8.56
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG13	3	8.56
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG11	9	8.56
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG12	9	8.56
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG13	9	8.56
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD11	4	8.55
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD12	4	8.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:544:A:THR:HG21	2:8:B:LEU:HD13	4	8.55
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD11	4	8.55
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD12	4	8.55
(1,22)	1:544:A:THR:HG22	2:8:B:LEU:HD13	4	8.55
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD11	4	8.55
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD12	4	8.55
(1,22)	1:544:A:THR:HG23	2:8:B:LEU:HD13	4	8.55
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG21	5	8.53
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG22	5	8.53
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG23	5	8.53
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG21	5	8.53
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG22	5	8.53
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG23	5	8.53
(3,1)	1:518:A:LEU:CG	2:6:C:LYS:H	7	8.49
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG11	3	8.49
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG12	3	8.49
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG13	3	8.49
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG11	3	8.49
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG12	3	8.49
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG13	3	8.49
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD11	9	8.47
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD12	9	8.47
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD13	9	8.47
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG11	6	8.46
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG12	6	8.46
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG13	6	8.46
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD11	8	8.46
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD12	8	8.46
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD13	8	8.46
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD11	9	8.44
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD12	9	8.44
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD13	9	8.44
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD21	9	8.44
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD22	9	8.44
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD23	9	8.44
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD11	5	8.44
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD12	5	8.44
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD13	5	8.44
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD11	3	8.42
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD12	3	8.42
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD13	3	8.42
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD11	3	8.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD12	3	8.42
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD13	3	8.42
(3,7)	1:518:A:LEU:CG	2:45:C:PHE:H	8	8.41
(3,1)	1:518:A:LEU:CG	2:6:C:LYS:H	10	8.4
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD11	10	8.39
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD12	10	8.39
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD13	10	8.39
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD21	10	8.39
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD22	10	8.39
(1,86)	1:512:A:ILE:HA	2:8:C:LEU:HD23	10	8.39
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD11	7	8.38
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD12	7	8.38
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD13	7	8.38
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD11	7	8.38
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD12	7	8.38
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD13	7	8.38
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD21	7	8.37
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD22	7	8.37
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD23	7	8.37
(1,6)	1:514:A:ALA:HB1	2:73:B:LEU:HG	9	8.37
(1,6)	1:514:A:ALA:HB2	2:73:B:LEU:HG	9	8.37
(1,6)	1:514:A:ALA:HB3	2:73:B:LEU:HG	9	8.37
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG21	7	8.36
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG22	7	8.36
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG23	7	8.36
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG21	7	8.36
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG22	7	8.36
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG23	7	8.36
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG21	3	8.35
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG22	3	8.35
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG23	3	8.35
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG21	3	8.35
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG22	3	8.35
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG23	3	8.35
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD11	6	8.35
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD12	6	8.35
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD13	6	8.35
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD11	6	8.35
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD12	6	8.35
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD13	6	8.35
(1,64)	1:548:A:ASP:OD1	2:42:B:ARG:NH2	5	8.35
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG11	8	8.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG12	8	8.35
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG13	8	8.35
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG11	8	8.35
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG12	8	8.35
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG13	8	8.35
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG11	8	8.35
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG12	8	8.35
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG13	8	8.35
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD11	4	8.33
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD12	4	8.33
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD13	4	8.33
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD11	4	8.33
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD12	4	8.33
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD13	4	8.33
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG11	9	8.32
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG12	9	8.32
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG13	9	8.32
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG11	9	8.32
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG12	9	8.32
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG13	9	8.32
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD11	5	8.32
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD12	5	8.32
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD13	5	8.32
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD11	5	8.32
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD12	5	8.32
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD13	5	8.32
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD11	5	8.32
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD12	5	8.32
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD13	5	8.32
(3,1)	1:518:A:LEU:CG	2:6:C:LYS:H	4	8.31
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG11	4	8.31
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG12	4	8.31
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG13	4	8.31
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG11	4	8.31
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG12	4	8.31
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG13	4	8.31
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG11	4	8.31
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG12	4	8.31
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG13	4	8.31
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG11	8	8.31
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG12	8	8.31
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG13	8	8.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG21	1	8.28
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG22	1	8.28
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG23	1	8.28
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG21	1	8.28
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG22	1	8.28
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG23	1	8.28
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG21	1	8.28
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG22	1	8.28
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG23	1	8.28
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD11	1	8.27
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD12	1	8.27
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD13	1	8.27
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD11	1	8.27
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD12	1	8.27
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD13	1	8.27
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD11	10	8.27
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD12	10	8.27
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD13	10	8.27
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD21	10	8.27
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD22	10	8.27
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD23	10	8.27
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG21	5	8.26
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG22	5	8.26
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG23	5	8.26
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG21	5	8.26
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG22	5	8.26
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG23	5	8.26
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG21	5	8.26
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG22	5	8.26
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG23	5	8.26
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG21	5	8.26
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG22	5	8.26
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG23	5	8.26
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG21	3	8.25
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG22	3	8.25
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG23	3	8.25
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG21	3	8.25
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG22	3	8.25
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG23	3	8.25
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG21	3	8.25
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG22	3	8.25
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG23	3	8.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG21	1	8.25
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG22	1	8.25
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG23	1	8.25
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG11	2	8.24
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG12	2	8.24
(1,24)	1:544:A:THR:HA	2:70:B:VAL:HG13	2	8.24
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG21	4	8.22
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG22	4	8.22
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG23	4	8.22
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG21	4	8.22
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG22	4	8.22
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG23	4	8.22
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD11	8	8.22
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD12	8	8.22
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD13	8	8.22
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD11	8	8.22
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD12	8	8.22
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD13	8	8.22
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD11	8	8.22
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD12	8	8.22
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD13	8	8.22
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG11	4	8.22
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG12	4	8.22
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG13	4	8.22
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG11	1	8.21
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG12	1	8.21
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG13	1	8.21
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG11	1	8.21
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG12	1	8.21
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG13	1	8.21
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG11	1	8.21
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG12	1	8.21
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG13	1	8.21
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD11	2	8.2
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD12	2	8.2
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD13	2	8.2
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD21	2	8.2
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD22	2	8.2
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD23	2	8.2
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD11	2	8.2
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD12	2	8.2
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD13	2	8.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD21	2	8.2
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD22	2	8.2
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD23	2	8.2
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG11	10	8.2
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG12	10	8.2
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG13	10	8.2
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG11	10	8.2
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG12	10	8.2
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG13	10	8.2
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG11	10	8.2
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG12	10	8.2
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG13	10	8.2
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG21	3	8.19
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG22	3	8.19
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG23	3	8.19
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD11	6	8.17
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD12	6	8.17
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD13	6	8.17
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD11	6	8.17
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD12	6	8.17
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD13	6	8.17
(3,13)	1:518:A:LEU:CG	2:68:C:HIS:H	8	8.16
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD11	7	8.16
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD12	7	8.16
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD13	7	8.16
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD11	7	8.16
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD12	7	8.16
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD13	7	8.16
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD11	7	8.16
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD12	7	8.16
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD13	7	8.16
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG21	7	8.16
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG22	7	8.16
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG23	7	8.16
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG21	7	8.15
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG22	7	8.15
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG23	7	8.15
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG21	7	8.15
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG22	7	8.15
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG23	7	8.15
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG21	7	8.15
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG22	7	8.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG23	7	8.15
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD21	3	8.15
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD22	3	8.15
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD23	3	8.15
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD21	3	8.15
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD22	3	8.15
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD23	3	8.15
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD21	3	8.15
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD22	3	8.15
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD23	3	8.15
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD21	8	8.14
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD22	8	8.14
(1,96)	1:515:A:SER:HB2	2:8:C:LEU:HD23	8	8.14
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD21	8	8.14
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD22	8	8.14
(1,96)	1:515:A:SER:HB3	2:8:C:LEU:HD23	8	8.14
(3,1)	1:518:A:LEU:CG	2:6:C:LYS:H	9	8.13
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD11	1	8.12
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD12	1	8.12
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD13	1	8.12
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD21	1	8.12
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD22	1	8.12
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD23	1	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD11	1	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD12	1	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD13	1	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD21	1	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD22	1	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD23	1	8.12
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD11	5	8.12
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD12	5	8.12
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD13	5	8.12
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD21	5	8.12
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD22	5	8.12
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD23	5	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD11	5	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD12	5	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD13	5	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD21	5	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD22	5	8.12
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD23	5	8.12
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD21	9	8.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD22	9	8.11
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD23	9	8.11
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD21	9	8.11
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD22	9	8.11
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD23	9	8.11
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD21	2	8.09
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD22	2	8.09
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD23	2	8.09
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD21	2	8.09
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD22	2	8.09
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD23	2	8.09
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG21	8	8.09
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG22	8	8.09
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG23	8	8.09
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG21	8	8.09
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG22	8	8.09
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG23	8	8.09
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG21	8	8.09
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG22	8	8.09
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG23	8	8.09
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG11	10	8.09
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG12	10	8.09
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG13	10	8.09
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG21	8	8.08
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG22	8	8.08
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG23	8	8.08
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG11	1	8.07
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG12	1	8.07
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG13	1	8.07
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG21	1	8.06
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG22	1	8.06
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG23	1	8.06
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG21	1	8.06
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG22	1	8.06
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG23	1	8.06
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG11	6	8.06
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG12	6	8.06
(1,84)	1:511:A:PRO:HG2	2:70:C:VAL:HG13	6	8.06
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG11	6	8.06
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG12	6	8.06
(1,84)	1:511:A:PRO:HG3	2:70:C:VAL:HG13	6	8.06
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD11	8	8.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD12	8	8.05
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD13	8	8.05
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD11	8	8.05
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD12	8	8.05
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD13	8	8.05
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD11	8	8.05
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD12	8	8.05
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD13	8	8.05
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD11	4	8.04
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD12	4	8.04
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD13	4	8.04
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD21	4	8.04
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD22	4	8.04
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD23	4	8.04
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD11	4	8.04
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD12	4	8.04
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD13	4	8.04
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD21	4	8.04
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD22	4	8.04
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD23	4	8.04
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD21	1	8.04
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD22	1	8.04
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD23	1	8.04
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD21	1	8.04
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD22	1	8.04
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD23	1	8.04
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG21	10	8.02
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG22	10	8.02
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG23	10	8.02
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG21	10	8.02
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG22	10	8.02
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG23	10	8.02
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG21	10	8.02
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG22	10	8.02
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG23	10	8.02
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG11	6	8.02
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG12	6	8.02
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG13	6	8.02
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG11	6	8.02
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG12	6	8.02
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG13	6	8.02
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG11	6	8.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG12	6	8.02
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG13	6	8.02
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG21	10	8.01
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG22	10	8.01
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG23	10	8.01
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG21	4	8.0
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG22	4	8.0
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG23	4	8.0
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG21	4	8.0
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG22	4	8.0
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG23	4	8.0
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG21	4	8.0
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG22	4	8.0
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG23	4	8.0
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD11	10	7.99
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD12	10	7.99
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD13	10	7.99
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD11	10	7.99
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD12	10	7.99
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD13	10	7.99
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD11	10	7.99
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD12	10	7.99
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD13	10	7.99
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG21	9	7.99
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG22	9	7.99
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG23	9	7.99
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG21	9	7.99
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG22	9	7.99
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG23	9	7.99
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG21	9	7.99
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG22	9	7.99
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG23	9	7.99
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG21	10	7.98
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG22	10	7.98
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG23	10	7.98
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG21	10	7.98
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG22	10	7.98
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG23	10	7.98
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD11	5	7.97
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD12	5	7.97
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD13	5	7.97
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD11	5	7.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD12	5	7.97
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD13	5	7.97
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD11	5	7.97
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD12	5	7.97
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD13	5	7.97
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG11	9	7.97
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG12	9	7.97
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG13	9	7.97
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG11	9	7.97
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG12	9	7.97
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG13	9	7.97
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG11	9	7.97
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG12	9	7.97
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG13	9	7.97
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG21	4	7.96
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG22	4	7.96
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG23	4	7.96
(3,10)	1:518:A:LEU:CG	2:51:C:GLU:H	2	7.92
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD11	3	7.89
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD12	3	7.89
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD13	3	7.89
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD21	3	7.89
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD22	3	7.89
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD23	3	7.89
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD11	3	7.89
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD12	3	7.89
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD13	3	7.89
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD21	3	7.89
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD22	3	7.89
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD23	3	7.89
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD11	6	7.89
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD12	6	7.89
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD13	6	7.89
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD11	6	7.89
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD12	6	7.89
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD13	6	7.89
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD11	6	7.89
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD12	6	7.89
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD13	6	7.89
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD11	7	7.89
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD12	7	7.89
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD13	7	7.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD21	7	7.89
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD22	7	7.89
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD23	7	7.89
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD11	9	7.89
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD12	9	7.89
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD13	9	7.89
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD21	9	7.89
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD22	9	7.89
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD23	9	7.89
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG21	6	7.88
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG22	6	7.88
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG23	6	7.88
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG21	6	7.88
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG22	6	7.88
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG23	6	7.88
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD11	8	7.86
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD12	8	7.86
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD13	8	7.86
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD11	8	7.86
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD12	8	7.86
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD13	8	7.86
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD11	8	7.86
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD12	8	7.86
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD13	8	7.86
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG21	6	7.83
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG22	6	7.83
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG23	6	7.83
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG21	6	7.83
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG22	6	7.83
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG23	6	7.83
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG21	6	7.83
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG22	6	7.83
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG23	6	7.83
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG21	9	7.83
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG22	9	7.83
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG23	9	7.83
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD11	7	7.82
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD12	7	7.82
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD13	7	7.82
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD21	7	7.82
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD22	7	7.82
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD23	7	7.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD11	7	7.82
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD12	7	7.82
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD13	7	7.82
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD21	7	7.82
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD22	7	7.82
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD23	7	7.82
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD11	4	7.81
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD12	4	7.81
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD13	4	7.81
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD21	4	7.81
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD22	4	7.81
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD23	4	7.81
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD11	5	7.81
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD12	5	7.81
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD13	5	7.81
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD21	5	7.81
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD22	5	7.81
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD23	5	7.81
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD11	10	7.78
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD12	10	7.78
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD13	10	7.78
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD21	10	7.78
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD22	10	7.78
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD23	10	7.78
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD11	10	7.78
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD12	10	7.78
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD13	10	7.78
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD21	10	7.78
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD22	10	7.78
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD23	10	7.78
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD11	7	7.78
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD12	7	7.78
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD13	7	7.78
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD11	7	7.78
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD12	7	7.78
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD13	7	7.78
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD11	7	7.78
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD12	7	7.78
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD13	7	7.78
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG21	2	7.77
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG22	2	7.77
(1,29)	1:544:A:THR:HG21	2:70:B:VAL:HG23	2	7.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG21	2	7.77
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG22	2	7.77
(1,29)	1:544:A:THR:HG22	2:70:B:VAL:HG23	2	7.77
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG21	2	7.77
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG22	2	7.77
(1,29)	1:544:A:THR:HG23	2:70:B:VAL:HG23	2	7.77
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG11	6	7.77
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG12	6	7.77
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG13	6	7.77
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD11	6	7.76
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD12	6	7.76
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD13	6	7.76
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD21	6	7.76
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD22	6	7.76
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD23	6	7.76
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD11	6	7.76
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD12	6	7.76
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD13	6	7.76
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD21	6	7.76
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD22	6	7.76
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD23	6	7.76
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG11	2	7.76
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG12	2	7.76
(1,28)	1:544:A:THR:HG21	2:70:B:VAL:HG13	2	7.76
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG11	2	7.76
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG12	2	7.76
(1,28)	1:544:A:THR:HG22	2:70:B:VAL:HG13	2	7.76
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG11	2	7.76
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG12	2	7.76
(1,28)	1:544:A:THR:HG23	2:70:B:VAL:HG13	2	7.76
(1,65)	1:552:A:GLU:OE2	2:42:B:ARG:NH1	3	7.75
(3,7)	1:518:A:LEU:CG	2:45:C:PHE:H	2	7.73
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD11	10	7.73
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD12	10	7.73
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD13	10	7.73
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD11	10	7.73
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD12	10	7.73
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD13	10	7.73
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD11	1	7.73
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD12	1	7.73
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD13	1	7.73
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD21	1	7.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD22	1	7.73
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD23	1	7.73
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD21	4	7.72
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD22	4	7.72
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD23	4	7.72
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD21	4	7.72
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD22	4	7.72
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD23	4	7.72
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD11	2	7.72
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD12	2	7.72
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD13	2	7.72
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD11	2	7.72
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD12	2	7.72
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD13	2	7.72
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD11	7	7.71
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD12	7	7.71
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD13	7	7.71
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD11	9	7.7
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD12	9	7.7
(1,95)	1:515:A:SER:HB2	2:8:C:LEU:HD13	9	7.7
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD11	9	7.7
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD12	9	7.7
(1,95)	1:515:A:SER:HB3	2:8:C:LEU:HD13	9	7.7
(3,7)	1:518:A:LEU:CG	2:45:C:PHE:H	3	7.69
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD21	6	7.69
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD22	6	7.69
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD23	6	7.69
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD21	6	7.69
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD22	6	7.69
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD23	6	7.69
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD11	1	7.67
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD12	1	7.67
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD13	1	7.67
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD11	1	7.67
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD12	1	7.67
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD13	1	7.67
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD11	1	7.67
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD12	1	7.67
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD13	1	7.67
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG11	9	7.67
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG12	9	7.67
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG13	9	7.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG21	2	7.65
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG22	2	7.65
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG23	2	7.65
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG21	6	7.64
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG22	6	7.64
(1,27)	1:544:A:THR:HB	2:70:B:VAL:HG23	6	7.64
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD11	9	7.63
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD12	9	7.63
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD13	9	7.63
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD21	9	7.63
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD22	9	7.63
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD23	9	7.63
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD11	9	7.63
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD12	9	7.63
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD13	9	7.63
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD21	9	7.63
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD22	9	7.63
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD23	9	7.63
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD11	5	7.63
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD12	5	7.63
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD13	5	7.63
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD11	5	7.63
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD12	5	7.63
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD13	5	7.63
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD11	5	7.63
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD12	5	7.63
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD13	5	7.63
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD11	10	7.61
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD12	10	7.61
(1,33)	1:545:A:SER:HA	2:73:B:LEU:HD13	10	7.61
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB2	8	7.6
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB3	8	7.6
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB2	8	7.6
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB3	8	7.6
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB2	8	7.6
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB3	8	7.6
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD11	8	7.59
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD12	8	7.59
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD13	8	7.59
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD21	8	7.59
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD22	8	7.59
(1,78)	1:511:A:PRO:HB2	2:8:C:LEU:HD23	8	7.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD11	8	7.59
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD12	8	7.59
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD13	8	7.59
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD21	8	7.59
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD22	8	7.59
(1,78)	1:511:A:PRO:HB3	2:8:C:LEU:HD23	8	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD11	3	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD12	3	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD13	3	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD21	3	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD22	3	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD23	3	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD11	6	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD12	6	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD13	6	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD21	6	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD22	6	7.59
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD23	6	7.59
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD11	4	7.58
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD12	4	7.58
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD13	4	7.58
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD11	4	7.58
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD12	4	7.58
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD13	4	7.58
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD11	4	7.58
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD12	4	7.58
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD13	4	7.58
(3,2)	1:518:A:LEU:CG	2:7:C:THR:H	8	7.57
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD11	1	7.57
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD12	1	7.57
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD13	1	7.57
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD11	1	7.57
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD12	1	7.57
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD13	1	7.57
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD11	9	7.54
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD12	9	7.54
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD13	9	7.54
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD11	9	7.54
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD12	9	7.54
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD13	9	7.54
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG11	2	7.53
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG12	2	7.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:544:A:THR:HB	2:70:B:VAL:HG13	2	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD11	2	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD12	2	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD13	2	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD21	2	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD22	2	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD23	2	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD11	8	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD12	8	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD13	8	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD21	8	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD22	8	7.53
(1,9)	1:543:A:THR:HA	2:8:B:LEU:HD23	8	7.53
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB2	3	7.49
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB3	3	7.49
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB2	3	7.49
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB3	3	7.49
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB2	3	7.49
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB3	3	7.49
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG11	2	7.48
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG12	2	7.48
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG13	2	7.48
(3,2)	1:518:A:LEU:CG	2:7:C:THR:H	3	7.47
(3,13)	1:518:A:LEU:CG	2:68:C:HIS:H	3	7.45
(1,65)	1:552:A:GLU:OE2	2:42:B:ARG:NH1	8	7.45
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG21	9	7.43
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG22	9	7.43
(1,98)	1:515:A:SER:HB2	2:70:C:VAL:HG23	9	7.43
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG21	9	7.43
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG22	9	7.43
(1,98)	1:515:A:SER:HB3	2:70:C:VAL:HG23	9	7.43
(3,13)	1:518:A:LEU:CG	2:68:C:HIS:H	1	7.42
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD21	7	7.41
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD22	7	7.41
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD23	7	7.41
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD21	7	7.41
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD22	7	7.41
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD23	7	7.41
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD11	2	7.38
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD12	2	7.38
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD13	2	7.38
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD21	2	7.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD22	2	7.38
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD23	2	7.38
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD11	2	7.38
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD12	2	7.38
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD13	2	7.38
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD21	2	7.38
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD22	2	7.38
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD23	2	7.38
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD11	2	7.38
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD12	2	7.38
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD13	2	7.38
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD21	2	7.38
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD22	2	7.38
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD23	2	7.38
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD11	3	7.33
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD12	3	7.33
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD13	3	7.33
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD21	3	7.33
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD22	3	7.33
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD23	3	7.33
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD11	3	7.33
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD12	3	7.33
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD13	3	7.33
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD21	3	7.33
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD22	3	7.33
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD23	3	7.33
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD11	3	7.33
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD12	3	7.33
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD13	3	7.33
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD21	3	7.33
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD22	3	7.33
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD23	3	7.33
(1,64)	1:548:A:ASP:OD2	2:42:B:ARG:NH2	10	7.33
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD11	9	7.32
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD12	9	7.32
(1,42)	1:551:A:LEU:HD21	2:44:B:ILE:HD13	9	7.32
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD11	9	7.32
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD12	9	7.32
(1,42)	1:551:A:LEU:HD22	2:44:B:ILE:HD13	9	7.32
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD11	9	7.32
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD12	9	7.32
(1,42)	1:551:A:LEU:HD23	2:44:B:ILE:HD13	9	7.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD11	7	7.28
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD12	7	7.28
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD13	7	7.28
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD21	7	7.28
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD22	7	7.28
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD23	7	7.28
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD11	7	7.28
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD12	7	7.28
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD13	7	7.28
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD21	7	7.28
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD22	7	7.28
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD23	7	7.28
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD11	7	7.28
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD12	7	7.28
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD13	7	7.28
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD21	7	7.28
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD22	7	7.28
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD23	7	7.28
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG11	7	7.28
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG12	7	7.28
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG13	7	7.28
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG21	7	7.28
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG22	7	7.28
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG23	7	7.28
(3,7)	1:518:A:LEU:CG	2:45:C:PHE:H	1	7.25
(3,13)	1:518:A:LEU:CG	2:68:C:HIS:H	2	7.23
(3,13)	1:518:A:LEU:CG	2:68:C:HIS:H	6	7.23
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD11	5	7.23
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD12	5	7.23
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD13	5	7.23
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD21	5	7.23
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD22	5	7.23
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD23	5	7.23
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD11	5	7.23
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD12	5	7.23
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD13	5	7.23
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD21	5	7.23
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD22	5	7.23
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD23	5	7.23
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD11	5	7.23
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD12	5	7.23
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD13	5	7.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD21	5	7.23
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD22	5	7.23
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD23	5	7.23
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD11	2	7.23
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD12	2	7.23
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD13	2	7.23
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD11	2	7.23
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD12	2	7.23
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD13	2	7.23
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD11	2	7.23
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD12	2	7.23
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD13	2	7.23
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD11	8	7.19
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD12	8	7.19
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD13	8	7.19
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD21	8	7.19
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD22	8	7.19
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD23	8	7.19
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD11	8	7.19
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD12	8	7.19
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD13	8	7.19
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD21	8	7.19
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD22	8	7.19
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD23	8	7.19
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD11	8	7.19
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD12	8	7.19
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD13	8	7.19
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD21	8	7.19
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD22	8	7.19
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD23	8	7.19
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG11	5	7.19
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG12	5	7.19
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG13	5	7.19
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG21	5	7.19
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG22	5	7.19
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG23	5	7.19
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB2	4	7.18
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB3	4	7.18
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB2	4	7.18
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB3	4	7.18
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB2	4	7.18
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB3	4	7.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,10)	1:518:A:LEU:CG	2:51:C:GLU:H	10	7.17
(3,2)	1:518:A:LEU:CG	2:7:C:THR:H	2	7.17
(1,64)	1:548:A:ASP:OD2	2:42:B:ARG:NH2	1	7.17
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD11	10	7.17
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD12	10	7.17
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD13	10	7.17
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD11	10	7.17
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD12	10	7.17
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD13	10	7.17
(3,7)	1:518:A:LEU:CG	2:45:C:PHE:H	5	7.16
(3,10)	1:518:A:LEU:CG	2:51:C:GLU:H	3	7.15
(3,10)	1:518:A:LEU:CG	2:51:C:GLU:H	1	7.13
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD11	1	7.13
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD12	1	7.13
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD13	1	7.13
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD21	1	7.13
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD22	1	7.13
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD23	1	7.13
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD11	1	7.13
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD12	1	7.13
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD13	1	7.13
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD21	1	7.13
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD22	1	7.13
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD23	1	7.13
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD11	1	7.13
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD12	1	7.13
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD13	1	7.13
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD21	1	7.13
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD22	1	7.13
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD23	1	7.13
(3,10)	1:518:A:LEU:CG	2:51:C:GLU:H	5	7.08
(1,6)	1:514:A:ALA:HB1	2:73:B:LEU:HG	7	7.08
(1,6)	1:514:A:ALA:HB2	2:73:B:LEU:HG	7	7.08
(1,6)	1:514:A:ALA:HB3	2:73:B:LEU:HG	7	7.08
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD21	5	7.08
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD22	5	7.08
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD23	5	7.08
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG11	5	7.06
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG12	5	7.06
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG13	5	7.06
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD11	3	7.05
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD12	3	7.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD13	3	7.05
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD11	3	7.05
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD12	3	7.05
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD13	3	7.05
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD11	3	7.05
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD12	3	7.05
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD13	3	7.05
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG11	1	7.02
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG12	1	7.02
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG13	1	7.02
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG21	1	7.02
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG22	1	7.02
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG23	1	7.02
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG11	8	7.0
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG12	8	7.0
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG13	8	7.0
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD11	4	7.0
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD12	4	7.0
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD13	4	7.0
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD21	4	7.0
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD22	4	7.0
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD23	4	7.0
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD11	4	7.0
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD12	4	7.0
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD13	4	7.0
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD21	4	7.0
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD22	4	7.0
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD23	4	7.0
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD11	4	7.0
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD12	4	7.0
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD13	4	7.0
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD21	4	7.0
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD22	4	7.0
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD23	4	7.0
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD11	3	7.0
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD12	3	7.0
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD13	3	7.0
(3,2)	1:518:A:LEU:CG	2:7:C:THR:H	6	6.99
(3,10)	1:518:A:LEU:CG	2:51:C:GLU:H	7	6.97
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG11	2	6.96
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG12	2	6.96
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG13	2	6.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG11	10	6.96
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG12	10	6.96
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG13	10	6.96
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG21	10	6.96
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG22	10	6.96
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG23	10	6.96
(3,7)	1:518:A:LEU:CG	2:45:C:PHE:H	7	6.93
(3,2)	1:518:A:LEU:CG	2:7:C:THR:H	1	6.93
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG11	4	6.93
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG12	4	6.93
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG13	4	6.93
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG21	4	6.93
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG22	4	6.93
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG23	4	6.93
(3,13)	1:518:A:LEU:CG	2:68:C:HIS:H	7	6.92
(1,64)	1:548:A:ASP:OD2	2:42:B:ARG:NH2	9	6.92
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG11	3	6.92
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG12	3	6.92
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG13	3	6.92
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG21	3	6.92
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG22	3	6.92
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG23	3	6.92
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG11	7	6.91
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG12	7	6.91
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG13	7	6.91
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD11	3	6.91
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD12	3	6.91
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD13	3	6.91
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD11	3	6.91
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD12	3	6.91
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD13	3	6.91
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD11	3	6.91
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD12	3	6.91
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD13	3	6.91
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG11	8	6.88
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG12	8	6.88
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG13	8	6.88
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG21	8	6.88
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG22	8	6.88
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG23	8	6.88
(3,13)	1:518:A:LEU:CG	2:68:C:HIS:H	10	6.87
(3,13)	1:518:A:LEU:CG	2:68:C:HIS:H	5	6.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG11	3	6.84
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG12	3	6.84
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG13	3	6.84
(3,2)	1:518:A:LEU:CG	2:7:C:THR:H	5	6.82
(1,6)	1:514:A:ALA:HB1	2:73:B:LEU:HG	4	6.81
(1,6)	1:514:A:ALA:HB2	2:73:B:LEU:HG	4	6.81
(1,6)	1:514:A:ALA:HB3	2:73:B:LEU:HG	4	6.81
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD11	4	6.81
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD12	4	6.81
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD13	4	6.81
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD11	6	6.8
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD12	6	6.8
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD13	6	6.8
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD21	6	6.8
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD22	6	6.8
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD23	6	6.8
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD11	6	6.8
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD12	6	6.8
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD13	6	6.8
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD21	6	6.8
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD22	6	6.8
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD23	6	6.8
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD11	6	6.8
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD12	6	6.8
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD13	6	6.8
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD21	6	6.8
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD22	6	6.8
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD23	6	6.8
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG11	8	6.75
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG12	8	6.75
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG13	8	6.75
(3,7)	1:518:A:LEU:CG	2:45:C:PHE:H	10	6.74
(1,65)	1:552:A:GLU:OE1	2:42:B:ARG:NH1	1	6.74
(1,3)	1:514:A:ALA:HB1	2:73:B:LEU:HA	3	6.74
(1,3)	1:514:A:ALA:HB2	2:73:B:LEU:HA	3	6.74
(1,3)	1:514:A:ALA:HB3	2:73:B:LEU:HA	3	6.74
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB2	6	6.73
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB3	6	6.73
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB2	6	6.73
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB3	6	6.73
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB2	6	6.73
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB3	6	6.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG11	4	6.71
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG12	4	6.71
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG13	4	6.71
(3,9)	1:518:A:LEU:CG	2:50:C:LEU:H	8	6.7
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG11	1	6.7
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG12	1	6.7
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG13	1	6.7
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG11	5	6.7
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG12	5	6.7
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG13	5	6.7
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD21	5	6.7
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD22	5	6.7
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD23	5	6.7
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD21	5	6.7
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD22	5	6.7
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD23	5	6.7
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD21	5	6.7
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD22	5	6.7
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD23	5	6.7
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG11	4	6.69
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG12	4	6.69
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG13	4	6.69
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG11	10	6.69
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG12	10	6.69
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG13	10	6.69
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG11	1	6.65
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG12	1	6.65
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG13	1	6.65
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG11	6	6.64
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG12	6	6.64
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG13	6	6.64
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG11	9	6.62
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG12	9	6.62
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG13	9	6.62
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG21	9	6.62
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG22	9	6.62
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG23	9	6.62
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD11	10	6.59
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD12	10	6.59
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD13	10	6.59
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD21	10	6.59
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD22	10	6.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD23	10	6.59
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD11	10	6.59
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD12	10	6.59
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD13	10	6.59
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD21	10	6.59
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD22	10	6.59
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD23	10	6.59
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD11	10	6.59
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD12	10	6.59
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD13	10	6.59
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD21	10	6.59
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD22	10	6.59
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD23	10	6.59
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG11	7	6.57
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG12	7	6.57
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG13	7	6.57
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD11	9	6.55
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD12	9	6.55
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD13	9	6.55
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD21	9	6.55
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD22	9	6.55
(1,87)	1:512:A:ILE:HG21	2:8:C:LEU:HD23	9	6.55
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD11	9	6.55
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD12	9	6.55
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD13	9	6.55
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD21	9	6.55
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD22	9	6.55
(1,87)	1:512:A:ILE:HG22	2:8:C:LEU:HD23	9	6.55
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD11	9	6.55
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD12	9	6.55
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD13	9	6.55
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD21	9	6.55
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD22	9	6.55
(1,87)	1:512:A:ILE:HG23	2:8:C:LEU:HD23	9	6.55
(3,13)	1:518:A:LEU:CG	2:68:C:HIS:H	4	6.53
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG11	10	6.53
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG12	10	6.53
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG13	10	6.53
(3,7)	1:518:A:LEU:CG	2:45:C:PHE:H	4	6.47
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD11	7	6.47
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD12	7	6.47
(1,35)	1:545:A:SER:HB2	2:73:B:LEU:HD13	7	6.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD11	7	6.47
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD12	7	6.47
(1,35)	1:545:A:SER:HB3	2:73:B:LEU:HD13	7	6.47
(3,10)	1:518:A:LEU:CG	2:51:C:GLU:H	4	6.45
(3,2)	1:518:A:LEU:CG	2:7:C:THR:H	7	6.45
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG11	2	6.44
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG12	2	6.44
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG13	2	6.44
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG11	2	6.44
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG12	2	6.44
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG13	2	6.44
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG11	3	6.44
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG12	3	6.44
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG13	3	6.44
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB2	5	6.43
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB3	5	6.43
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB2	5	6.43
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB3	5	6.43
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB2	5	6.43
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB3	5	6.43
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB2	10	6.43
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB3	10	6.43
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB2	10	6.43
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB3	10	6.43
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB2	10	6.43
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB3	10	6.43
(3,8)	1:518:A:LEU:CG	2:49:C:GLN:H	8	6.41
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD21	10	6.41
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD22	10	6.41
(1,34)	1:545:A:SER:HA	2:73:B:LEU:HD23	10	6.41
(3,10)	1:518:A:LEU:CG	2:51:C:GLU:H	6	6.4
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG11	2	6.39
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG12	2	6.39
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG13	2	6.39
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG21	2	6.39
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG22	2	6.39
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG23	2	6.39
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD11	4	6.39
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD12	4	6.39
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD13	4	6.39
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD11	4	6.39
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD12	4	6.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD13	4	6.39
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD11	4	6.39
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD12	4	6.39
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD13	4	6.39
(3,2)	1:518:A:LEU:CG	2:7:C:THR:H	4	6.37
(3,2)	1:518:A:LEU:CG	2:7:C:THR:H	9	6.37
(1,6)	1:514:A:ALA:HB1	2:73:B:LEU:HG	6	6.34
(1,6)	1:514:A:ALA:HB2	2:73:B:LEU:HG	6	6.34
(1,6)	1:514:A:ALA:HB3	2:73:B:LEU:HG	6	6.34
(1,3)	1:514:A:ALA:HB1	2:73:B:LEU:HA	4	6.34
(1,3)	1:514:A:ALA:HB2	2:73:B:LEU:HA	4	6.34
(1,3)	1:514:A:ALA:HB3	2:73:B:LEU:HA	4	6.34
(3,7)	1:518:A:LEU:CG	2:45:C:PHE:H	6	6.33
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG11	8	6.33
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG12	8	6.33
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG13	8	6.33
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG11	8	6.33
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG12	8	6.33
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG13	8	6.33
(3,2)	1:518:A:LEU:CG	2:7:C:THR:H	10	6.29
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG11	5	6.28
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG12	5	6.28
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG13	5	6.28
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG11	5	6.28
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG12	5	6.28
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG13	5	6.28
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG11	6	6.21
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG12	6	6.21
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG13	6	6.21
(1,6)	1:514:A:ALA:HB1	2:73:B:LEU:HG	10	6.17
(1,6)	1:514:A:ALA:HB2	2:73:B:LEU:HG	10	6.17
(1,6)	1:514:A:ALA:HB3	2:73:B:LEU:HG	10	6.17
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD21	8	6.17
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD22	8	6.17
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD23	8	6.17
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD21	8	6.17
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD22	8	6.17
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD23	8	6.17
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD21	8	6.17
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD22	8	6.17
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD23	8	6.17
(1,64)	1:548:A:ASP:OD2	2:42:B:ARG:NH2	2	6.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD11	6	6.14
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD12	6	6.14
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD13	6	6.14
(3,9)	1:518:A:LEU:CG	2:50:C:LEU:H	2	6.12
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG11	3	6.12
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG12	3	6.12
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG13	3	6.12
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG11	3	6.12
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG12	3	6.12
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG13	3	6.12
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG11	9	6.11
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG12	9	6.11
(1,82)	1:511:A:PRO:HA	2:70:C:VAL:HG13	9	6.11
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG11	7	6.1
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG12	7	6.1
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG13	7	6.1
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG11	7	6.1
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG12	7	6.1
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG13	7	6.1
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD21	8	6.09
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD22	8	6.09
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD23	8	6.09
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD21	2	6.05
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD22	2	6.05
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD23	2	6.05
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD21	2	6.05
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD22	2	6.05
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD23	2	6.05
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD21	2	6.05
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD22	2	6.05
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD23	2	6.05
(3,8)	1:518:A:LEU:CG	2:49:C:GLN:H	2	6.04
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD11	6	6.03
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD12	6	6.03
(1,41)	1:551:A:LEU:HD11	2:44:B:ILE:HD13	6	6.03
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD11	6	6.03
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD12	6	6.03
(1,41)	1:551:A:LEU:HD12	2:44:B:ILE:HD13	6	6.03
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD11	6	6.03
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD12	6	6.03
(1,41)	1:551:A:LEU:HD13	2:44:B:ILE:HD13	6	6.03
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG11	9	6.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG12	9	6.02
(1,93)	1:515:A:SER:HA	2:70:C:VAL:HG13	9	6.02
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG11	6	6.02
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG12	6	6.02
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG13	6	6.02
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG21	6	6.02
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG22	6	6.02
(1,40)	1:548:A:ASP:HA	2:70:B:VAL:HG23	6	6.02
(1,3)	1:514:A:ALA:HB1	2:73:B:LEU:HA	8	6.02
(1,3)	1:514:A:ALA:HB2	2:73:B:LEU:HA	8	6.02
(1,3)	1:514:A:ALA:HB3	2:73:B:LEU:HA	8	6.02
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD11	6	6.0
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD12	6	6.0
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD13	6	6.0
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD11	6	6.0
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD12	6	6.0
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD13	6	6.0
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD11	6	6.0
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD12	6	6.0
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD13	6	6.0
(1,6)	1:514:A:ALA:HB1	2:73:B:LEU:HG	1	5.99
(1,6)	1:514:A:ALA:HB2	2:73:B:LEU:HG	1	5.99
(1,6)	1:514:A:ALA:HB3	2:73:B:LEU:HG	1	5.99
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG11	4	5.97
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG12	4	5.97
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG13	4	5.97
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG11	4	5.97
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG12	4	5.97
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG13	4	5.97
(3,7)	1:518:A:LEU:CG	2:45:C:PHE:H	9	5.95
(3,14)	1:518:A:LEU:CG	2:69:C:LEU:H	8	5.9
(3,6)	1:518:A:LEU:CG	2:44:C:ILE:H	8	5.86
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG11	6	5.85
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG12	6	5.85
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG13	6	5.85
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG11	6	5.85
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG12	6	5.85
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG13	6	5.85
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG11	1	5.82
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG12	1	5.82
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG13	1	5.82
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG11	1	5.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG12	1	5.82
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG13	1	5.82
(1,65)	1:552:A:GLU:OE1	2:42:B:ARG:NH1	5	5.82
(1,3)	1:514:A:ALA:HB1	2:73:B:LEU:HA	2	5.79
(1,3)	1:514:A:ALA:HB2	2:73:B:LEU:HA	2	5.79
(1,3)	1:514:A:ALA:HB3	2:73:B:LEU:HA	2	5.79
(3,13)	1:518:A:LEU:CG	2:68:C:HIS:H	9	5.78
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD21	10	5.78
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD22	10	5.78
(1,36)	1:545:A:SER:HB2	2:73:B:LEU:HD23	10	5.78
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD21	10	5.78
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD22	10	5.78
(1,36)	1:545:A:SER:HB3	2:73:B:LEU:HD23	10	5.78
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG11	10	5.77
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG12	10	5.77
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG13	10	5.77
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG11	10	5.77
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG12	10	5.77
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG13	10	5.77
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD21	9	5.73
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD22	9	5.73
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD23	9	5.73
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD21	9	5.73
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD22	9	5.73
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD23	9	5.73
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD21	9	5.73
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD22	9	5.73
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD23	9	5.73
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD11	5	5.72
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD12	5	5.72
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD13	5	5.72
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD21	5	5.72
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD22	5	5.72
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD23	5	5.72
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD11	5	5.72
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD12	5	5.72
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD13	5	5.72
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD21	5	5.72
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD22	5	5.72
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD23	5	5.72
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD21	1	5.67
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD22	1	5.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD23	1	5.67
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD21	1	5.67
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD22	1	5.67
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD23	1	5.67
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD21	1	5.67
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD22	1	5.67
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD23	1	5.67
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB2	2	5.62
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB3	2	5.62
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB2	2	5.62
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB3	2	5.62
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB2	2	5.62
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB3	2	5.62
(1,65)	1:552:A:GLU:OE1	2:42:B:ARG:NH1	9	5.61
(1,3)	1:514:A:ALA:HB1	2:73:B:LEU:HA	10	5.55
(1,3)	1:514:A:ALA:HB2	2:73:B:LEU:HA	10	5.55
(1,3)	1:514:A:ALA:HB3	2:73:B:LEU:HA	10	5.55
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB2	1	5.54
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB3	1	5.54
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB2	1	5.54
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB3	1	5.54
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB2	1	5.54
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB3	1	5.54
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD11	1	5.51
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD12	1	5.51
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD13	1	5.51
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD11	1	5.51
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD12	1	5.51
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD13	1	5.51
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD11	1	5.51
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD12	1	5.51
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD13	1	5.51
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD21	2	5.47
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD22	2	5.47
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD23	2	5.47
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD21	6	5.45
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD22	6	5.45
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD23	6	5.45
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD21	6	5.45
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD22	6	5.45
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD23	6	5.45
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD21	6	5.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD22	6	5.45
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD23	6	5.45
(3,10)	1:518:A:LEU:CG	2:51:C:GLU:H	9	5.44
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD11	2	5.43
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD12	2	5.43
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD13	2	5.43
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD11	2	5.43
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD12	2	5.43
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD13	2	5.43
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD11	2	5.43
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD12	2	5.43
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD13	2	5.43
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD11	3	5.41
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD12	3	5.41
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD13	3	5.41
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD21	3	5.41
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD22	3	5.41
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD23	3	5.41
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD11	3	5.41
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD12	3	5.41
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD13	3	5.41
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD21	3	5.41
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD22	3	5.41
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD23	3	5.41
(1,3)	1:514:A:ALA:HB1	2:73:B:LEU:HA	6	5.41
(1,3)	1:514:A:ALA:HB2	2:73:B:LEU:HA	6	5.41
(1,3)	1:514:A:ALA:HB3	2:73:B:LEU:HA	6	5.41
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD21	1	5.4
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD22	1	5.4
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD23	1	5.4
(3,14)	1:518:A:LEU:CG	2:69:C:LEU:H	2	5.31
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB2	9	5.29
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB3	9	5.29
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB2	9	5.29
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB3	9	5.29
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB2	9	5.29
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB3	9	5.29
(1,3)	1:514:A:ALA:HB1	2:73:B:LEU:HA	9	5.26
(1,3)	1:514:A:ALA:HB2	2:73:B:LEU:HA	9	5.26
(1,3)	1:514:A:ALA:HB3	2:73:B:LEU:HA	9	5.26
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD21	9	5.24
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD22	9	5.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD23	9	5.24
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG11	9	5.16
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG12	9	5.16
(1,97)	1:515:A:SER:HB2	2:70:C:VAL:HG13	9	5.16
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG11	9	5.16
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG12	9	5.16
(1,97)	1:515:A:SER:HB3	2:70:C:VAL:HG13	9	5.16
(3,9)	1:518:A:LEU:CG	2:50:C:LEU:H	10	5.15
(3,6)	1:518:A:LEU:CG	2:44:C:ILE:H	3	5.15
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD21	4	5.15
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD22	4	5.15
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD23	4	5.15
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD21	4	5.15
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD22	4	5.15
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD23	4	5.15
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD21	4	5.15
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD22	4	5.15
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD23	4	5.15
(1,65)	1:552:A:GLU:OE2	2:42:B:ARG:NH1	10	5.12
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD21	6	5.12
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD22	6	5.12
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD23	6	5.12
(3,6)	1:518:A:LEU:CG	2:44:C:ILE:H	2	5.11
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD11	9	5.1
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD12	9	5.1
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD13	9	5.1
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD11	9	5.1
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD12	9	5.1
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD13	9	5.1
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD11	9	5.1
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD12	9	5.1
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD13	9	5.1
(3,9)	1:518:A:LEU:CG	2:50:C:LEU:H	1	5.08
(3,14)	1:518:A:LEU:CG	2:69:C:LEU:H	3	5.07
(3,9)	1:518:A:LEU:CG	2:50:C:LEU:H	7	5.06
(1,3)	1:514:A:ALA:HB1	2:73:B:LEU:HA	5	5.06
(1,3)	1:514:A:ALA:HB2	2:73:B:LEU:HA	5	5.06
(1,3)	1:514:A:ALA:HB3	2:73:B:LEU:HA	5	5.06
(3,9)	1:518:A:LEU:CG	2:50:C:LEU:H	3	5.04
(3,6)	1:518:A:LEU:CG	2:44:C:ILE:H	1	5.03
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD21	4	4.99
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD22	4	4.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD23	4	4.99
(3,8)	1:518:A:LEU:CG	2:49:C:GLN:H	3	4.98
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD11	1	4.98
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD12	1	4.98
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD13	1	4.98
(3,14)	1:518:A:LEU:CG	2:69:C:LEU:H	5	4.96
(3,9)	1:518:A:LEU:CG	2:50:C:LEU:H	5	4.94
(3,6)	1:518:A:LEU:CG	2:44:C:ILE:H	5	4.94
(3,8)	1:518:A:LEU:CG	2:49:C:GLN:H	7	4.87
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD11	10	4.87
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD12	10	4.87
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD13	10	4.87
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD11	10	4.87
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD12	10	4.87
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD13	10	4.87
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD11	10	4.87
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD12	10	4.87
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD13	10	4.87
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD11	8	4.86
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD12	8	4.86
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD13	8	4.86
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD21	8	4.86
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD22	8	4.86
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD23	8	4.86
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD11	8	4.86
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD12	8	4.86
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD13	8	4.86
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD21	8	4.86
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD22	8	4.86
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD23	8	4.86
(3,8)	1:518:A:LEU:CG	2:49:C:GLN:H	1	4.75
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD11	2	4.73
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD12	2	4.73
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD13	2	4.73
(3,8)	1:518:A:LEU:CG	2:49:C:GLN:H	5	4.72
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD11	9	4.65
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD12	9	4.65
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD13	9	4.65
(3,14)	1:518:A:LEU:CG	2:69:C:LEU:H	7	4.64
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB2	7	4.64
(1,7)	1:514:A:ALA:HB1	2:73:B:LEU:HB3	7	4.64
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB2	7	4.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:514:A:ALA:HB2	2:73:B:LEU:HB3	7	4.64
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB2	7	4.64
(1,7)	1:514:A:ALA:HB3	2:73:B:LEU:HB3	7	4.64
(3,6)	1:518:A:LEU:CG	2:44:C:ILE:H	7	4.61
(3,6)	1:518:A:LEU:CG	2:44:C:ILE:H	6	4.59
(1,3)	1:514:A:ALA:HB1	2:73:B:LEU:HA	1	4.59
(1,3)	1:514:A:ALA:HB2	2:73:B:LEU:HA	1	4.59
(1,3)	1:514:A:ALA:HB3	2:73:B:LEU:HA	1	4.59
(1,101)	1:516:A:THR:HG21	2:73:C:LEU:HA	4	4.57
(1,101)	1:516:A:THR:HG22	2:73:C:LEU:HA	4	4.57
(1,101)	1:516:A:THR:HG23	2:73:C:LEU:HA	4	4.57
(3,6)	1:518:A:LEU:CG	2:44:C:ILE:H	10	4.56
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD21	7	4.52
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD22	7	4.52
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD23	7	4.52
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD21	7	4.52
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD22	7	4.52
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD23	7	4.52
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD21	7	4.52
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD22	7	4.52
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD23	7	4.52
(1,3)	1:514:A:ALA:HB1	2:73:B:LEU:HA	7	4.5
(1,3)	1:514:A:ALA:HB2	2:73:B:LEU:HA	7	4.5
(1,3)	1:514:A:ALA:HB3	2:73:B:LEU:HA	7	4.5
(3,14)	1:518:A:LEU:CG	2:69:C:LEU:H	4	4.49
(3,9)	1:518:A:LEU:CG	2:50:C:LEU:H	6	4.43
(3,14)	1:518:A:LEU:CG	2:69:C:LEU:H	6	4.42
(3,8)	1:518:A:LEU:CG	2:49:C:GLN:H	10	4.42
(3,5)	1:518:A:LEU:CG	2:43:C:LEU:H	8	4.4
(3,14)	1:518:A:LEU:CG	2:69:C:LEU:H	1	4.35
(3,9)	1:518:A:LEU:CG	2:50:C:LEU:H	4	4.33
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD11	10	4.28
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD12	10	4.28
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD13	10	4.28
(1,101)	1:516:A:THR:HG21	2:73:C:LEU:HA	1	4.23
(1,101)	1:516:A:THR:HG22	2:73:C:LEU:HA	1	4.23
(1,101)	1:516:A:THR:HG23	2:73:C:LEU:HA	1	4.23
(1,101)	1:516:A:THR:HG21	2:73:C:LEU:HA	9	4.21
(1,101)	1:516:A:THR:HG22	2:73:C:LEU:HA	9	4.21
(1,101)	1:516:A:THR:HG23	2:73:C:LEU:HA	9	4.21
(3,6)	1:518:A:LEU:CG	2:44:C:ILE:H	4	4.19
(3,4)	1:518:A:LEU:CG	2:9:C:THR:H	6	4.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,14)	1:518:A:LEU:CG	2:69:C:LEU:H	10	4.05
(3,14)	1:518:A:LEU:CG	2:69:C:LEU:H	9	4.04
(3,9)	1:518:A:LEU:CG	2:50:C:LEU:H	9	3.87
(3,4)	1:518:A:LEU:CG	2:9:C:THR:H	5	3.87
(3,6)	1:518:A:LEU:CG	2:44:C:ILE:H	9	3.8
(3,5)	1:518:A:LEU:CG	2:43:C:LEU:H	2	3.8
(1,101)	1:516:A:THR:HG21	2:73:C:LEU:HA	3	3.77
(1,101)	1:516:A:THR:HG22	2:73:C:LEU:HA	3	3.77
(1,101)	1:516:A:THR:HG23	2:73:C:LEU:HA	3	3.77
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD11	4	3.71
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD12	4	3.71
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD13	4	3.71
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD21	4	3.71
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD22	4	3.71
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD23	4	3.71
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD11	4	3.71
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD12	4	3.71
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD13	4	3.71
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD21	4	3.71
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD22	4	3.71
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD23	4	3.71
(3,8)	1:518:A:LEU:CG	2:49:C:GLN:H	4	3.66
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD11	1	3.61
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD12	1	3.61
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD13	1	3.61
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD21	1	3.61
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD22	1	3.61
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD23	1	3.61
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD11	1	3.61
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD12	1	3.61
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD13	1	3.61
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD21	1	3.61
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD22	1	3.61
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD23	1	3.61
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD11	7	3.57
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD12	7	3.57
(1,4)	1:514:A:ALA:HB1	2:73:B:LEU:HD13	7	3.57
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD11	7	3.57
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD12	7	3.57
(1,4)	1:514:A:ALA:HB2	2:73:B:LEU:HD13	7	3.57
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD11	7	3.57
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD12	7	3.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:514:A:ALA:HB3	2:73:B:LEU:HD13	7	3.57
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD21	7	3.57
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD22	7	3.57
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD23	7	3.57
(3,8)	1:518:A:LEU:CG	2:49:C:GLN:H	9	3.46
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD21	10	3.45
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD22	10	3.45
(1,5)	1:514:A:ALA:HB1	2:73:B:LEU:HD23	10	3.45
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD21	10	3.45
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD22	10	3.45
(1,5)	1:514:A:ALA:HB2	2:73:B:LEU:HD23	10	3.45
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD21	10	3.45
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD22	10	3.45
(1,5)	1:514:A:ALA:HB3	2:73:B:LEU:HD23	10	3.45
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD11	6	3.42
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD12	6	3.42
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD13	6	3.42
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD21	6	3.42
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD22	6	3.42
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD23	6	3.42
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD11	6	3.42
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD12	6	3.42
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD13	6	3.42
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD21	6	3.42
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD22	6	3.42
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD23	6	3.42
(1,65)	1:552:A:GLU:OE2	2:42:B:ARG:NH1	2	3.39
(3,8)	1:518:A:LEU:CG	2:49:C:GLN:H	6	3.36
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD11	2	3.33
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD12	2	3.33
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD13	2	3.33
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD21	2	3.33
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD22	2	3.33
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD23	2	3.33
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD11	2	3.33
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD12	2	3.33
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD13	2	3.33
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD21	2	3.33
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD22	2	3.33
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD23	2	3.33
(3,3)	1:518:A:LEU:CG	2:8:C:LEU:H	8	3.14
(1,101)	1:516:A:THR:HG21	2:73:C:LEU:HA	10	3.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,101)	1:516:A:THR:HG22	2:73:C:LEU:HA	10	3.12
(1,101)	1:516:A:THR:HG23	2:73:C:LEU:HA	10	3.12
(3,5)	1:518:A:LEU:CG	2:43:C:LEU:H	3	3.1
(1,101)	1:516:A:THR:HG21	2:73:C:LEU:HA	8	3.05
(1,101)	1:516:A:THR:HG22	2:73:C:LEU:HA	8	3.05
(1,101)	1:516:A:THR:HG23	2:73:C:LEU:HA	8	3.05
(3,4)	1:518:A:LEU:CG	2:9:C:THR:H	8	3.03
(1,101)	1:516:A:THR:HG21	2:73:C:LEU:HA	5	3.01
(1,101)	1:516:A:THR:HG22	2:73:C:LEU:HA	5	3.01
(1,101)	1:516:A:THR:HG23	2:73:C:LEU:HA	5	3.01
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD11	9	2.99
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD12	9	2.99
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD13	9	2.99
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD21	9	2.99
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD22	9	2.99
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD23	9	2.99
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD11	9	2.99
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD12	9	2.99
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD13	9	2.99
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD21	9	2.99
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD22	9	2.99
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD23	9	2.99
(3,5)	1:518:A:LEU:CG	2:43:C:LEU:H	10	2.96
(3,3)	1:518:A:LEU:CG	2:8:C:LEU:H	3	2.95
(3,5)	1:518:A:LEU:CG	2:43:C:LEU:H	5	2.93
(1,101)	1:516:A:THR:HG21	2:73:C:LEU:HA	6	2.91
(1,101)	1:516:A:THR:HG22	2:73:C:LEU:HA	6	2.91
(1,101)	1:516:A:THR:HG23	2:73:C:LEU:HA	6	2.91
(3,5)	1:518:A:LEU:CG	2:43:C:LEU:H	1	2.85
(3,4)	1:518:A:LEU:CG	2:9:C:THR:H	3	2.82
(3,3)	1:518:A:LEU:CG	2:8:C:LEU:H	2	2.8
(3,4)	1:518:A:LEU:CG	2:9:C:THR:H	2	2.78
(3,5)	1:518:A:LEU:CG	2:43:C:LEU:H	7	2.74
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD21	10	2.72
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD22	10	2.72
(1,2)	1:514:A:ALA:HA	2:73:B:LEU:HD23	10	2.72
(3,5)	1:518:A:LEU:CG	2:43:C:LEU:H	6	2.69
(3,3)	1:518:A:LEU:CG	2:8:C:LEU:H	1	2.62
(3,3)	1:518:A:LEU:CG	2:8:C:LEU:H	6	2.61
(1,254)	1:515:A:SER:HA	1:518:A:LEU:H	6	2.58
(1,254)	1:515:A:SER:HA	1:518:A:LEU:H	4	2.57
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD11	7	2.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD12	7	2.51
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD13	7	2.51
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD21	7	2.51
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD22	7	2.51
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD23	7	2.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD11	7	2.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD12	7	2.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD13	7	2.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD21	7	2.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD22	7	2.51
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD23	7	2.51
(1,101)	1:516:A:THR:HG21	2:73:C:LEU:HA	2	2.48
(1,101)	1:516:A:THR:HG22	2:73:C:LEU:HA	2	2.48
(1,101)	1:516:A:THR:HG23	2:73:C:LEU:HA	2	2.48
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD12	3	2.45
(3,15)	1:518:A:LEU:CG	2:70:C:VAL:H	8	2.41
(3,4)	1:518:A:LEU:CG	2:9:C:THR:H	7	2.4
(3,3)	1:518:A:LEU:CG	2:8:C:LEU:H	5	2.39
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD13	10	2.39
(3,5)	1:518:A:LEU:CG	2:43:C:LEU:H	4	2.35
(1,254)	1:515:A:SER:HA	1:518:A:LEU:H	9	2.24
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD11	7	2.23
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD12	7	2.23
(1,1)	1:514:A:ALA:HA	2:73:B:LEU:HD13	7	2.23
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD22	8	2.19
(1,254)	1:515:A:SER:HA	1:518:A:LEU:H	10	2.18
(1,254)	1:515:A:SER:HA	1:518:A:LEU:H	1	2.15
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD13	9	2.13
(3,3)	1:518:A:LEU:CG	2:8:C:LEU:H	7	2.08
(1,1388)	1:599:A:ILE:HD11	1:562:A:TRP:HH2	7	2.06
(3,3)	1:518:A:LEU:CG	2:8:C:LEU:H	4	1.99
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD21	7	1.98
(3,3)	1:518:A:LEU:CG	2:8:C:LEU:H	9	1.96
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD11	1	1.95
(3,4)	1:518:A:LEU:CG	2:9:C:THR:H	1	1.94
(3,4)	1:518:A:LEU:CG	2:9:C:THR:H	4	1.93
(3,3)	1:518:A:LEU:CG	2:8:C:LEU:H	10	1.93
(3,5)	1:518:A:LEU:CG	2:43:C:LEU:H	9	1.91
(1,3018)	2:40:C:GLN:HG3	2:71:C:LEU:HD22	5	1.83
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD11	10	1.81
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD12	10	1.81
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD13	10	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD21	10	1.81
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD22	10	1.81
(1,39)	1:548:A:ASP:HB2	2:73:B:LEU:HD23	10	1.81
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD11	10	1.81
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD12	10	1.81
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD13	10	1.81
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD21	10	1.81
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD22	10	1.81
(1,39)	1:548:A:ASP:HB3	2:73:B:LEU:HD23	10	1.81
(1,498)	1:573:A:LEU:H	1:575:A:MET:H	5	1.78
(1,498)	1:573:A:LEU:H	1:575:A:MET:H	1	1.74
(1,1388)	1:599:A:ILE:HD13	1:562:A:TRP:HZ3	10	1.71
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD21	6	1.7
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD23	9	1.7
(1,498)	1:573:A:LEU:H	1:575:A:MET:H	6	1.69
(3,15)	1:518:A:LEU:CG	2:70:C:VAL:H	2	1.67
(1,498)	1:573:A:LEU:H	1:575:A:MET:H	10	1.67
(1,101)	1:516:A:THR:HG21	2:73:C:LEU:HA	7	1.67
(1,101)	1:516:A:THR:HG22	2:73:C:LEU:HA	7	1.67
(1,101)	1:516:A:THR:HG23	2:73:C:LEU:HA	7	1.67
(2,4)	1:484:A:LYS:O	1:488:A:ALA:N	4	1.66
(2,3)	1:484:A:LYS:O	1:488:A:ALA:H	4	1.64
(1,3714)	2:1:B:MET:HE3	2:17:B:VAL:HG13	5	1.63
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD23	9	1.61
(1,1448)	2:1:C:MET:HE2	2:17:C:VAL:HG13	3	1.54
(3,4)	1:518:A:LEU:CG	2:9:C:THR:H	9	1.52
(1,3018)	2:40:C:GLN:HG3	2:71:C:LEU:HD22	2	1.49
(1,1448)	2:1:C:MET:HE2	2:17:C:VAL:HG11	5	1.47
(1,254)	1:515:A:SER:HA	1:518:A:LEU:H	8	1.46
(1,3714)	2:1:B:MET:HE1	2:17:B:VAL:HG13	1	1.45
(3,15)	1:518:A:LEU:CG	2:70:C:VAL:H	3	1.42
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	7	1.42
(1,3714)	2:1:B:MET:HE1	2:17:B:VAL:HG11	6	1.39
(1,1448)	2:1:C:MET:HE3	2:17:C:VAL:HG13	4	1.39
(1,1448)	2:1:C:MET:HE2	2:17:C:VAL:HG12	9	1.38
(1,3714)	2:1:B:MET:HE2	2:17:B:VAL:HG11	8	1.36
(1,3018)	2:40:C:GLN:HG2	2:71:C:LEU:HD13	4	1.36
(1,1448)	2:1:C:MET:HE3	2:17:C:VAL:HG11	10	1.36
(1,3714)	2:1:B:MET:HE1	2:17:B:VAL:HG11	3	1.35
(1,1448)	2:1:C:MET:HE1	2:17:C:VAL:HG13	1	1.35
(1,3714)	2:1:B:MET:HE1	2:17:B:VAL:HG12	7	1.34
(3,209)	2:27:B:LYS:HE2	2:69:B:LEU:HD12	5	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,4)	1:518:A:LEU:CG	2:9:C:THR:H	10	1.33
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	7	1.33
(1,1510)	2:1:C:MET:HE3	2:67:C:LEU:HD12	4	1.33
(1,498)	1:573:A:LEU:H	1:575:A:MET:H	3	1.33
(1,3632)	2:70:C:VAL:HG11	2:68:C:HIS:HB3	10	1.32
(1,3714)	2:1:B:MET:HE3	2:17:B:VAL:HG11	9	1.31
(1,1448)	2:1:C:MET:HE3	2:17:C:VAL:HG12	7	1.31
(2,4)	1:484:A:LYS:O	1:488:A:ALA:N	7	1.3
(1,498)	1:573:A:LEU:H	1:575:A:MET:H	4	1.3
(1,1448)	2:1:C:MET:HE2	2:17:C:VAL:HG11	2	1.29
(1,1448)	2:1:C:MET:HE2	2:17:C:VAL:HG11	6	1.29
(1,1388)	1:599:A:ILE:HD11	1:562:A:TRP:HH2	4	1.29
(1,5284)	2:40:B:GLN:HG3	2:71:B:LEU:HD23	7	1.28
(1,498)	1:573:A:LEU:H	1:575:A:MET:H	8	1.27
(1,3632)	2:66:C:THR:HG22	2:68:C:HIS:HB3	7	1.26
(1,3714)	2:1:B:MET:HE3	2:17:B:VAL:HG11	4	1.25
(1,3713)	2:1:B:MET:HE3	2:17:B:VAL:HG13	5	1.25
(2,3)	1:484:A:LYS:O	1:488:A:ALA:H	7	1.24
(1,3714)	2:1:B:MET:HE1	2:17:B:VAL:HG11	10	1.23
(1,498)	1:573:A:LEU:H	1:575:A:MET:H	7	1.23
(1,3632)	2:70:C:VAL:HG11	2:68:C:HIS:HB3	5	1.22
(1,1448)	2:1:C:MET:HE1	2:17:C:VAL:HG12	8	1.22
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	9	1.21
(1,100)	1:516:A:THR:HG21	2:72:C:ARG:HD2	8	1.21
(1,100)	1:516:A:THR:HG21	2:72:C:ARG:HD3	8	1.21
(1,100)	1:516:A:THR:HG22	2:72:C:ARG:HD2	8	1.21
(1,100)	1:516:A:THR:HG22	2:72:C:ARG:HD3	8	1.21
(1,100)	1:516:A:THR:HG23	2:72:C:ARG:HD2	8	1.21
(1,100)	1:516:A:THR:HG23	2:72:C:ARG:HD3	8	1.21
(1,3714)	2:1:B:MET:HE3	2:17:B:VAL:HG13	2	1.2
(1,3632)	2:66:C:THR:HG23	2:68:C:HIS:HB3	1	1.19
(1,3632)	2:70:C:VAL:HG12	2:68:C:HIS:HB3	9	1.18
(1,1839)	2:6:C:LYS:HG3	2:66:C:THR:HG21	1	1.18
(1,498)	1:573:A:LEU:H	1:575:A:MET:H	9	1.17
(3,15)	1:518:A:LEU:CG	2:70:C:VAL:H	5	1.16
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD12	3	1.16
(1,1447)	2:1:C:MET:HE2	2:17:C:VAL:HG13	3	1.16
(1,498)	1:573:A:LEU:H	1:575:A:MET:H	2	1.16
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD22	4	1.14
(1,863)	1:520:A:ILE:HG13	1:562:A:TRP:HE3	10	1.14
(1,3776)	2:1:B:MET:HE1	2:67:B:LEU:HD11	6	1.13
(1,1839)	2:6:C:LYS:HG2	2:66:C:THR:HG23	8	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	1:484:A:LYS:O	1:488:A:ALA:N	1	1.11
(2,4)	1:484:A:LYS:O	1:488:A:ALA:N	2	1.11
(1,254)	1:515:A:SER:HA	1:518:A:LEU:H	5	1.11
(3,15)	1:518:A:LEU:CG	2:70:C:VAL:H	6	1.1
(2,4)	1:484:A:LYS:O	1:488:A:ALA:N	10	1.1
(1,5284)	2:40:B:GLN:HG3	2:71:B:LEU:HD21	3	1.1
(1,1447)	2:1:C:MET:HE2	2:17:C:VAL:HG11	5	1.09
(1,3713)	2:1:B:MET:HE1	2:17:B:VAL:HG13	1	1.07
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	10	1.07
(1,261)	1:516:A:THR:HA	1:518:A:LEU:H	6	1.07
(3,15)	1:518:A:LEU:CG	2:70:C:VAL:H	1	1.06
(1,4105)	2:6:B:LYS:HG3	2:66:B:THR:HG23	5	1.06
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	3	1.06
(1,5284)	2:40:B:GLN:HG3	2:71:B:LEU:HD21	6	1.05
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD22	4	1.05
(1,5183)	2:36:B:ILE:HG21	2:71:B:LEU:HD12	7	1.05
(2,3)	1:484:A:LYS:O	1:488:A:ALA:H	1	1.04
(2,3)	1:484:A:LYS:O	1:488:A:ALA:H	2	1.04
(1,4105)	2:6:B:LYS:HG3	2:66:B:THR:HG23	4	1.04
(1,3632)	2:66:C:THR:HG22	2:68:C:HIS:HB3	3	1.04
(3,89)	2:27:C:LYS:HE2	2:69:C:LEU:HD12	9	1.03
(1,3632)	2:66:C:THR:HG21	2:68:C:HIS:HB3	6	1.03
(2,3)	1:484:A:LYS:O	1:488:A:ALA:H	10	1.02
(1,4105)	2:6:B:LYS:HG3	2:66:B:THR:HG23	10	1.02
(1,3632)	2:70:C:VAL:HG12	2:68:C:HIS:HB3	2	1.02
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD11	1	1.02
(1,1447)	2:1:C:MET:HE3	2:17:C:VAL:HG13	4	1.02
(1,1388)	1:599:A:ILE:HD12	1:562:A:TRP:HZ3	1	1.02
(1,5309)	2:41:B:GLN:H	2:69:B:LEU:HD13	6	1.01
(1,4745)	2:40:B:GLN:HG2	2:39:B:ASP:H	8	1.01
(1,4105)	2:6:B:LYS:HG3	2:66:B:THR:HG23	2	1.01
(1,3713)	2:1:B:MET:HE1	2:17:B:VAL:HG11	6	1.01
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	10	1.01
(1,1839)	2:6:C:LYS:HG3	2:66:C:THR:HG23	3	1.01
(1,5284)	2:40:B:GLN:HG3	2:71:B:LEU:HD23	4	1.0
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	6	1.0
(1,4105)	2:6:B:LYS:HG3	2:66:B:THR:HG21	7	1.0
(1,1447)	2:1:C:MET:HE2	2:17:C:VAL:HG12	9	1.0
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD22	8	0.99
(1,3713)	2:1:B:MET:HE2	2:17:B:VAL:HG11	8	0.98
(1,3632)	2:66:C:THR:HG23	2:68:C:HIS:HB3	4	0.98
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD22	2	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1447)	2:1:C:MET:HE3	2:17:C:VAL:HG11	10	0.98
(1,3713)	2:1:B:MET:HE1	2:17:B:VAL:HG11	3	0.97
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	3	0.97
(1,1447)	2:1:C:MET:HE1	2:17:C:VAL:HG13	1	0.97
(1,3713)	2:1:B:MET:HE1	2:17:B:VAL:HG12	7	0.96
(1,4105)	2:6:B:LYS:HG3	2:66:B:THR:HG21	1	0.95
(1,254)	1:515:A:SER:HA	1:518:A:LEU:H	2	0.94
(1,3713)	2:1:B:MET:HE3	2:17:B:VAL:HG11	9	0.93
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD11	1	0.93
(1,1839)	2:6:C:LYS:HG3	2:66:C:THR:HG23	7	0.93
(1,1447)	2:1:C:MET:HE3	2:17:C:VAL:HG12	7	0.93
(3,259)	2:66:B:THR:HG21	2:67:B:LEU:HD21	2	0.92
(3,15)	1:518:A:LEU:CG	2:70:C:VAL:H	10	0.92
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	10	0.92
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	6	0.91
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	9	0.91
(1,1447)	2:1:C:MET:HE2	2:17:C:VAL:HG11	2	0.91
(1,1447)	2:1:C:MET:HE2	2:17:C:VAL:HG11	6	0.91
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD22	8	0.9
(3,15)	1:518:A:LEU:CG	2:70:C:VAL:H	7	0.89
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD22	2	0.89
(1,1510)	2:1:C:MET:HE1	2:67:C:LEU:HD12	3	0.89
(1,3017)	2:40:C:GLN:HB2	2:71:C:LEU:HD23	9	0.88
(1,3713)	2:1:B:MET:HE3	2:17:B:VAL:HG11	4	0.87
(1,1837)	2:6:C:LYS:HG3	2:66:C:THR:HG21	1	0.87
(1,4014)	2:5:B:VAL:HG21	2:13:B:ILE:HG13	7	0.86
(1,3713)	2:1:B:MET:HE1	2:17:B:VAL:HG11	10	0.86
(3,259)	2:66:B:THR:HG21	2:67:B:LEU:HD21	3	0.85
(1,3757)	2:1:B:MET:HE3	2:56:B:LEU:HD13	2	0.85
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD23	6	0.85
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD12	3	0.85
(1,863)	1:520:A:ILE:HG13	1:562:A:TRP:HD1	6	0.85
(1,5360)	2:43:B:LEU:HD22	2:67:B:LEU:HB3	6	0.84
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD11	9	0.84
(1,1447)	2:1:C:MET:HE1	2:17:C:VAL:HG12	8	0.84
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	8	0.83
(1,3713)	2:1:B:MET:HE3	2:17:B:VAL:HG13	2	0.83
(1,1510)	2:1:C:MET:HE2	2:67:C:LEU:HD11	9	0.83
(1,120)	1:503:A:ASP:H	1:506:A:LEU:H	10	0.83
(1,3776)	2:1:B:MET:HE3	2:67:B:LEU:HD13	1	0.82
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD12	7	0.82
(1,261)	1:516:A:THR:HA	1:518:A:LEU:H	4	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1837)	2:6:C:LYS:HG2	2:66:C:THR:HG23	8	0.81
(3,259)	2:66:B:THR:HG21	2:67:B:LEU:HD21	9	0.8
(3,139)	2:66:C:THR:HG22	2:67:C:LEU:HD21	9	0.8
(1,5309)	2:41:B:GLN:H	2:69:B:LEU:HD13	8	0.8
(1,3757)	2:1:B:MET:HE1	2:56:B:LEU:HD11	3	0.8
(3,259)	2:66:B:THR:HG22	2:67:B:LEU:HD21	8	0.79
(1,3757)	2:1:B:MET:HE3	2:56:B:LEU:HD11	4	0.79
(1,1839)	2:6:C:LYS:HG3	2:66:C:THR:HG22	4	0.79
(3,259)	2:66:B:THR:HG23	2:67:B:LEU:HD22	1	0.78
(2,4)	1:484:A:LYS:O	1:488:A:ALA:N	6	0.78
(1,4105)	2:6:B:LYS:HG3	2:66:B:THR:HG23	6	0.78
(1,3776)	2:1:B:MET:HE3	2:67:B:LEU:HD13	5	0.78
(1,3632)	2:66:C:THR:HG23	2:68:C:HIS:HB3	8	0.78
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD23	4	0.78
(1,5108)	2:34:B:GLU:HG3	2:69:B:LEU:HD21	3	0.77
(1,4031)	2:17:B:VAL:HG12	2:29:B:LYS:HG2	4	0.77
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD22	1	0.77
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD22	9	0.77
(1,1160)	1:563:A:VAL:HG12	1:562:A:TRP:HZ2	7	0.77
(1,248)	1:515:A:SER:H	1:517:A:ASP:H	5	0.77
(3,259)	2:66:B:THR:HG23	2:67:B:LEU:HD21	7	0.76
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG11	9	0.76
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	10	0.76
(1,1838)	2:6:C:LYS:HG3	2:66:C:THR:HG21	1	0.76
(1,1491)	2:1:C:MET:HE3	2:56:C:LEU:HD11	7	0.76
(1,4103)	2:6:B:LYS:HG3	2:66:B:THR:HG23	5	0.75
(1,3094)	2:43:C:LEU:HD21	2:67:C:LEU:HB3	9	0.75
(1,1835)	2:6:C:LYS:HE3	2:66:C:THR:HG23	9	0.75
(1,1748)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	8	0.75
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	8	0.74
(1,5183)	2:36:B:ILE:HG22	2:71:B:LEU:HD23	8	0.74
(1,4014)	2:5:B:VAL:HG22	2:13:B:ILE:HG13	10	0.74
(1,1491)	2:1:C:MET:HE3	2:56:C:LEU:HD12	10	0.74
(1,863)	1:520:A:ILE:HG12	1:562:A:TRP:HE3	1	0.74
(1,4103)	2:6:B:LYS:HG3	2:66:B:THR:HG23	4	0.73
(1,3015)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	9	0.73
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	8	0.73
(2,3)	1:484:A:LYS:O	1:488:A:ALA:H	6	0.72
(1,2917)	2:36:C:ILE:HG23	2:71:C:LEU:HD21	3	0.72
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG13	7	0.71
(1,3776)	2:1:B:MET:HE2	2:67:B:LEU:HD12	2	0.71
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD22	5	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1565)	2:3:C:ILE:HD11	2:3:C:ILE:HA	3	0.71
(1,1510)	2:1:C:MET:HE2	2:67:C:LEU:HD13	7	0.71
(1,1161)	1:563:A:VAL:HG21	1:562:A:TRP:HZ2	4	0.71
(1,4103)	2:6:B:LYS:HG3	2:66:B:THR:HG23	2	0.7
(1,4103)	2:6:B:LYS:HG3	2:66:B:THR:HG23	10	0.7
(1,4014)	2:5:B:VAL:HG23	2:13:B:ILE:HG13	4	0.7
(1,4012)	2:5:B:VAL:HG21	2:13:B:ILE:HG13	7	0.7
(1,3831)	2:3:B:ILE:HD11	2:3:B:ILE:HA	3	0.7
(1,1838)	2:6:C:LYS:HG2	2:66:C:THR:HG23	8	0.7
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD23	10	0.7
(1,1565)	2:3:C:ILE:HD13	2:3:C:ILE:HA	6	0.7
(1,120)	1:503:A:ASP:H	1:506:A:LEU:H	7	0.7
(3,139)	2:66:C:THR:HG22	2:67:C:LEU:HD12	7	0.69
(1,4103)	2:6:B:LYS:HG3	2:66:B:THR:HG21	7	0.69
(1,3757)	2:1:B:MET:HE3	2:56:B:LEU:HD12	9	0.69
(1,2917)	2:36:C:ILE:HG21	2:71:C:LEU:HD23	9	0.69
(1,1837)	2:6:C:LYS:HG3	2:66:C:THR:HG23	3	0.69
(1,1565)	2:3:C:ILE:HD11	2:3:C:ILE:HA	1	0.69
(1,1565)	2:3:C:ILE:HD11	2:3:C:ILE:HA	2	0.69
(1,1510)	2:1:C:MET:HE1	2:67:C:LEU:HD11	2	0.69
(1,5309)	2:41:B:GLN:H	2:69:B:LEU:HD11	7	0.68
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD12	2	0.68
(1,3831)	2:3:B:ILE:HD12	2:3:B:ILE:HA	6	0.68
(1,3015)	2:40:C:GLN:HB3	2:71:C:LEU:HD12	3	0.68
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	2	0.68
(1,253)	1:515:A:SER:HA	1:517:A:ASP:H	5	0.68
(1,248)	1:515:A:SER:H	1:517:A:ASP:H	8	0.68
(1,5109)	2:34:B:GLU:HG3	2:69:B:LEU:HD21	3	0.67
(1,3831)	2:3:B:ILE:HD12	2:3:B:ILE:HA	5	0.67
(1,3756)	2:1:B:MET:HE3	2:56:B:LEU:HD13	2	0.67
(1,1565)	2:3:C:ILE:HD13	2:3:C:ILE:HA	5	0.67
(1,412)	1:547:A:MET:HE1	1:548:A:ASP:H	8	0.67
(1,412)	1:547:A:MET:HE2	1:548:A:ASP:H	8	0.67
(1,412)	1:547:A:MET:HE3	1:548:A:ASP:H	8	0.67
(1,261)	1:516:A:THR:HA	1:518:A:LEU:H	9	0.67
(1,5360)	2:43:B:LEU:HD21	2:67:B:LEU:HB3	1	0.66
(1,5108)	2:34:B:GLU:HG3	2:69:B:LEU:HD23	6	0.66
(1,3776)	2:1:B:MET:HE3	2:67:B:LEU:HD11	7	0.66
(1,3016)	2:40:C:GLN:HB2	2:71:C:LEU:HD23	9	0.66
(1,4101)	2:6:B:LYS:HE2	2:66:B:THR:HG23	8	0.65
(1,3831)	2:3:B:ILE:HD12	2:3:B:ILE:HA	1	0.65
(1,3831)	2:3:B:ILE:HD11	2:3:B:ILE:HA	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2917)	2:36:C:ILE:HG21	2:71:C:LEU:HD11	1	0.65
(1,1839)	2:6:C:LYS:HG3	2:66:C:THR:HG22	5	0.65
(1,1565)	2:3:C:ILE:HD12	2:3:C:ILE:HA	9	0.65
(1,1491)	2:1:C:MET:HE2	2:56:C:LEU:HD13	2	0.65
(1,261)	1:516:A:THR:HA	1:518:A:LEU:H	1	0.65
(3,153)	2:3:B:ILE:HG22	2:67:B:LEU:HG	6	0.64
(1,4104)	2:6:B:LYS:HG3	2:66:B:THR:HG23	5	0.64
(1,4103)	2:6:B:LYS:HG3	2:66:B:THR:HG21	1	0.64
(1,3831)	2:3:B:ILE:HD11	2:3:B:ILE:HA	8	0.64
(1,1565)	2:3:C:ILE:HD11	2:3:C:ILE:HA	7	0.64
(1,1491)	2:1:C:MET:HE1	2:56:C:LEU:HD12	8	0.64
(1,5184)	2:36:B:ILE:HG21	2:71:B:LEU:HD12	7	0.63
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD12	2	0.63
(1,3831)	2:3:B:ILE:HD11	2:3:B:ILE:HA	4	0.63
(1,3800)	2:2:B:GLN:HE22	2:14:B:THR:HG21	4	0.63
(1,3756)	2:1:B:MET:HE1	2:56:B:LEU:HD11	3	0.63
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD11	5	0.63
(1,1491)	2:1:C:MET:HE2	2:56:C:LEU:HD11	6	0.63
(1,1491)	2:1:C:MET:HE3	2:56:C:LEU:HD12	9	0.63
(1,5309)	2:41:B:GLN:H	2:71:B:LEU:HD22	5	0.62
(1,5309)	2:41:B:GLN:H	2:69:B:LEU:HD12	10	0.62
(1,5284)	2:40:B:GLN:HG3	2:71:B:LEU:HD22	5	0.62
(1,5284)	2:40:B:GLN:HG3	2:71:B:LEU:HD23	8	0.62
(1,4104)	2:6:B:LYS:HG3	2:66:B:THR:HG23	4	0.62
(1,3831)	2:3:B:ILE:HD12	2:3:B:ILE:HA	7	0.62
(1,3831)	2:3:B:ILE:HD11	2:3:B:ILE:HA	9	0.62
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG12	5	0.62
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG13	8	0.62
(1,3776)	2:1:B:MET:HE2	2:67:B:LEU:HD12	9	0.62
(1,3757)	2:1:B:MET:HE1	2:56:B:LEU:HD11	6	0.62
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD22	5	0.62
(1,2842)	2:34:C:GLU:HG3	2:69:C:LEU:HD12	1	0.62
(1,1565)	2:3:C:ILE:HD13	2:3:C:ILE:HA	4	0.62
(1,505)	1:575:A:MET:HE1	1:575:A:MET:H	6	0.62
(1,505)	1:575:A:MET:HE2	1:575:A:MET:H	6	0.62
(1,505)	1:575:A:MET:HE3	1:575:A:MET:H	6	0.62
(3,24)	2:1:C:MET:HE3	2:67:C:LEU:HD12	4	0.61
(2,4)	1:484:A:LYS:O	1:488:A:ALA:N	3	0.61
(1,5309)	2:41:B:GLN:H	2:71:B:LEU:HD13	4	0.61
(1,3756)	2:1:B:MET:HE3	2:56:B:LEU:HD11	4	0.61
(1,2842)	2:34:C:GLU:HG3	2:69:C:LEU:HD21	4	0.61
(1,1837)	2:6:C:LYS:HG3	2:66:C:THR:HG23	7	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,863)	1:520:A:ILE:HG13	1:562:A:TRP:HD1	5	0.61
(3,33)	2:3:C:ILE:HG22	2:67:C:LEU:HG	4	0.6
(1,5283)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	7	0.6
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD21	3	0.6
(1,4745)	2:40:B:GLN:HG2	2:39:B:ASP:H	9	0.6
(1,4337)	2:15:B:LEU:HD13	2:33:B:LYS:HD2	7	0.6
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG13	1	0.6
(1,3094)	2:43:C:LEU:HD21	2:67:C:LEU:HB3	8	0.6
(1,2917)	2:36:C:ILE:HG21	2:71:C:LEU:HD21	10	0.6
(3,139)	2:66:C:THR:HG23	2:67:C:LEU:HD23	1	0.59
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD12	2	0.59
(1,4104)	2:6:B:LYS:HG3	2:66:B:THR:HG23	2	0.59
(1,4104)	2:6:B:LYS:HG3	2:66:B:THR:HG23	10	0.59
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	7	0.59
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	5	0.59
(1,1746)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	8	0.59
(1,1620)	2:29:C:LYS:HA	2:33:C:LYS:HE2	6	0.59
(1,1533)	2:68:C:HIS:HA	2:5:C:VAL:HG11	6	0.59
(1,505)	1:575:A:MET:HE1	1:575:A:MET:H	10	0.59
(1,505)	1:575:A:MET:HE2	1:575:A:MET:H	10	0.59
(1,505)	1:575:A:MET:HE3	1:575:A:MET:H	10	0.59
(1,412)	1:547:A:MET:HE1	1:548:A:ASP:H	4	0.59
(1,412)	1:547:A:MET:HE2	1:548:A:ASP:H	4	0.59
(1,412)	1:547:A:MET:HE3	1:548:A:ASP:H	4	0.59
(1,120)	1:503:A:ASP:H	1:506:A:LEU:H	1	0.59
(3,15)	1:518:A:LEU:CG	2:70:C:VAL:H	4	0.58
(1,5360)	2:43:B:LEU:HD22	2:67:B:LEU:HB3	7	0.58
(1,5284)	2:40:B:GLN:HG3	2:71:B:LEU:HD12	2	0.58
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD22	5	0.58
(1,4104)	2:6:B:LYS:HG3	2:66:B:THR:HG21	7	0.58
(1,4012)	2:5:B:VAL:HG22	2:13:B:ILE:HG13	10	0.58
(1,3831)	2:3:B:ILE:HD12	2:3:B:ILE:HA	10	0.58
(1,3048)	2:42:C:ARG:HA	2:69:C:LEU:HD22	9	0.58
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD12	2	0.58
(1,3015)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	10	0.58
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD11	1	0.58
(1,1838)	2:6:C:LYS:HG3	2:66:C:THR:HG23	3	0.58
(1,1490)	2:1:C:MET:HE3	2:56:C:LEU:HD11	7	0.58
(1,5183)	2:36:B:ILE:HG22	2:71:B:LEU:HD11	2	0.57
(1,5108)	2:34:B:GLU:HG3	2:69:B:LEU:HD23	4	0.57
(1,4230)	2:13:B:ILE:HG22	2:15:B:LEU:HD22	5	0.57
(1,4105)	2:6:B:LYS:HG3	2:66:B:THR:HG21	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD13	4	0.57
(1,1565)	2:3:C:ILE:HD12	2:3:C:ILE:HA	10	0.57
(1,5300)	2:41:B:GLN:HA	2:71:B:LEU:HD21	5	0.56
(1,5109)	2:34:B:GLU:HG3	2:69:B:LEU:HD23	6	0.56
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG11	10	0.56
(1,1490)	2:1:C:MET:HE3	2:56:C:LEU:HD12	10	0.56
(1,505)	1:575:A:MET:HE1	1:575:A:MET:H	8	0.56
(1,505)	1:575:A:MET:HE2	1:575:A:MET:H	8	0.56
(1,505)	1:575:A:MET:HE3	1:575:A:MET:H	8	0.56
(1,5898)	2:70:B:VAL:HG12	2:68:B:HIS:HB3	9	0.55
(1,4012)	2:5:B:VAL:HG23	2:13:B:ILE:HG13	4	0.55
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD12	7	0.55
(1,1748)	2:5:C:VAL:HG21	2:15:C:LEU:HG	3	0.55
(1,1491)	2:1:C:MET:HE3	2:56:C:LEU:HD12	4	0.55
(1,412)	1:547:A:MET:HE1	1:548:A:ASP:H	10	0.55
(1,412)	1:547:A:MET:HE2	1:548:A:ASP:H	10	0.55
(1,412)	1:547:A:MET:HE3	1:548:A:ASP:H	10	0.55
(3,33)	2:3:C:ILE:HG23	2:67:C:LEU:HG	8	0.54
(1,5898)	2:70:B:VAL:HG11	2:68:B:HIS:HB3	10	0.54
(1,5183)	2:36:B:ILE:HG22	2:71:B:LEU:HD23	5	0.54
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG12	3	0.54
(1,1565)	2:3:C:ILE:HD13	2:3:C:ILE:HA	8	0.54
(1,5309)	2:41:B:GLN:H	2:69:B:LEU:HD12	3	0.53
(1,5300)	2:41:B:GLN:HA	2:69:B:LEU:HD13	6	0.53
(1,4104)	2:6:B:LYS:HG3	2:66:B:THR:HG21	1	0.53
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD22	3	0.53
(1,2843)	2:34:C:GLU:HG3	2:69:C:LEU:HD12	1	0.53
(1,1804)	2:11:C:LYS:HG3	2:10:C:GLY:HA3	6	0.53
(1,1765)	2:17:C:VAL:HG13	2:29:C:LYS:HG3	9	0.53
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD22	1	0.53
(1,412)	1:547:A:MET:HE1	1:548:A:ASP:H	9	0.53
(1,412)	1:547:A:MET:HE2	1:548:A:ASP:H	9	0.53
(1,412)	1:547:A:MET:HE3	1:548:A:ASP:H	9	0.53
(1,261)	1:516:A:THR:HA	1:518:A:LEU:H	10	0.53
(1,5299)	2:41:B:GLN:HA	2:71:B:LEU:HD21	5	0.52
(1,5107)	2:34:B:GLU:HG3	2:36:B:ILE:HG13	3	0.52
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG21	3	0.52
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG21	3	0.52
(1,4014)	2:5:B:VAL:HG23	2:15:B:LEU:HG	1	0.52
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD21	7	0.52
(1,1533)	2:68:C:HIS:HA	2:5:C:VAL:HG11	7	0.52
(3,89)	2:27:C:LYS:HE2	2:69:C:LEU:HD11	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:484:A:LYS:O	1:488:A:ALA:H	3	0.51
(1,5309)	2:41:B:GLN:H	2:71:B:LEU:HD11	1	0.51
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD21	3	0.51
(1,5183)	2:36:B:ILE:HG22	2:71:B:LEU:HD23	10	0.51
(1,4147)	2:7:B:THR:HA	2:69:B:LEU:HD23	2	0.51
(1,4046)	2:5:B:VAL:HG12	2:67:B:LEU:HB2	5	0.51
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG21	8	0.51
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG21	8	0.51
(1,4031)	2:17:B:VAL:HG11	2:29:B:LYS:HG3	2	0.51
(1,3756)	2:1:B:MET:HE3	2:56:B:LEU:HD12	9	0.51
(1,2843)	2:34:C:GLU:HG3	2:69:C:LEU:HD21	4	0.51
(1,2054)	2:15:C:LEU:HD21	2:29:C:LYS:HG2	9	0.51
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD21	7	0.51
(1,412)	1:547:A:MET:HE1	1:548:A:ASP:H	3	0.51
(1,412)	1:547:A:MET:HE2	1:548:A:ASP:H	3	0.51
(1,412)	1:547:A:MET:HE3	1:548:A:ASP:H	3	0.51
(3,153)	2:3:B:ILE:HG23	2:67:B:LEU:HG	5	0.5
(3,34)	2:3:C:ILE:HG13	2:67:C:LEU:HB2	10	0.5
(1,3033)	2:41:C:GLN:HA	2:69:C:LEU:HD12	7	0.5
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	7	0.5
(1,2842)	2:34:C:GLU:HG3	2:69:C:LEU:HD23	5	0.5
(1,1838)	2:6:C:LYS:HG3	2:66:C:THR:HG23	7	0.5
(1,1620)	2:29:C:LYS:HA	2:33:C:LYS:HE2	9	0.5
(1,120)	1:503:A:ASP:H	1:506:A:LEU:H	2	0.5
(1,5299)	2:41:B:GLN:HA	2:69:B:LEU:HD13	6	0.49
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD12	1	0.49
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD22	5	0.49
(1,3776)	2:1:B:MET:HE3	2:67:B:LEU:HD12	3	0.49
(1,3776)	2:1:B:MET:HE1	2:67:B:LEU:HD12	8	0.49
(1,1994)	2:36:C:ILE:HG13	2:34:C:GLU:HG3	4	0.49
(1,1510)	2:1:C:MET:HE2	2:67:C:LEU:HD11	5	0.49
(1,5277)	2:40:B:GLN:HB3	2:71:B:LEU:HD23	7	0.48
(1,5183)	2:36:B:ILE:HG23	2:71:B:LEU:HD23	6	0.48
(1,1839)	2:6:C:LYS:HG3	2:66:C:THR:HG21	2	0.48
(1,1839)	2:6:C:LYS:HG3	2:66:C:THR:HG21	9	0.48
(1,1837)	2:6:C:LYS:HG3	2:66:C:THR:HG22	4	0.48
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD21	3	0.48
(1,863)	1:520:A:ILE:HG13	1:562:A:TRP:HD1	9	0.48
(1,99)	1:516:A:THR:HG21	2:72:C:ARG:HG2	8	0.48
(1,99)	1:516:A:THR:HG21	2:72:C:ARG:HG3	8	0.48
(1,99)	1:516:A:THR:HG22	2:72:C:ARG:HG2	8	0.48
(1,99)	1:516:A:THR:HG22	2:72:C:ARG:HG3	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:516:A:THR:HG23	2:72:C:ARG:HG2	8	0.48
(1,99)	1:516:A:THR:HG23	2:72:C:ARG:HG3	8	0.48
(1,5109)	2:34:B:GLU:HG3	2:69:B:LEU:HD23	4	0.47
(1,4103)	2:6:B:LYS:HG3	2:66:B:THR:HG23	6	0.47
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG21	5	0.47
(1,3757)	2:1:B:MET:HE1	2:56:B:LEU:HD11	10	0.47
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	6	0.47
(1,2054)	2:15:C:LEU:HD23	2:29:C:LYS:HG2	4	0.47
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD22	2	0.47
(1,1533)	2:2:C:GLN:HA	2:17:C:VAL:HG13	4	0.47
(1,1533)	2:68:C:HIS:HA	2:5:C:VAL:HG13	8	0.47
(1,1490)	2:1:C:MET:HE2	2:56:C:LEU:HD13	2	0.47
(1,1388)	1:599:A:ILE:HD11	1:562:A:TRP:HZ3	8	0.47
(1,863)	1:520:A:ILE:HG12	1:562:A:TRP:HE3	2	0.47
(1,4100)	2:6:B:LYS:HD2	2:66:B:THR:HG21	6	0.46
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG21	4	0.46
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG21	5	0.46
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG21	4	0.46
(1,4030)	2:17:B:VAL:HG12	2:29:B:LYS:HG2	4	0.46
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG12	4	0.46
(1,3048)	2:42:C:ARG:HA	2:69:C:LEU:HD22	1	0.46
(1,2050)	2:15:C:LEU:HD11	2:29:C:LYS:HA	9	0.46
(1,1510)	2:1:C:MET:HE3	2:67:C:LEU:HD13	1	0.46
(1,1490)	2:1:C:MET:HE2	2:56:C:LEU:HD11	6	0.46
(1,1490)	2:1:C:MET:HE1	2:56:C:LEU:HD12	8	0.46
(3,89)	2:27:C:LYS:HE2	2:69:C:LEU:HD11	1	0.45
(1,5300)	2:41:B:GLN:HA	2:71:B:LEU:HD11	1	0.45
(1,4047)	2:5:B:VAL:HG12	2:67:B:LEU:HB2	5	0.45
(1,1490)	2:1:C:MET:HE3	2:56:C:LEU:HD12	9	0.45
(1,5309)	2:41:B:GLN:H	2:71:B:LEU:HD11	2	0.44
(1,4031)	2:17:B:VAL:HG11	2:29:B:LYS:HG3	5	0.44
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD13	1	0.44
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD13	6	0.44
(1,3756)	2:1:B:MET:HE1	2:56:B:LEU:HD11	6	0.44
(1,3014)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	9	0.44
(1,1836)	2:6:C:LYS:HG3	2:66:C:THR:HG21	1	0.44
(1,5314)	2:42:B:ARG:HA	2:69:B:LEU:HD21	5	0.43
(1,3757)	2:1:B:MET:HE1	2:56:B:LEU:HD13	7	0.43
(1,2054)	2:15:C:LEU:HD22	2:29:C:LYS:HG2	2	0.43
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD11	3	0.43
(3,144)	2:1:B:MET:HE1	2:67:B:LEU:HD11	6	0.42
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD11	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3800)	2:2:B:GLN:HE22	2:14:B:THR:HG23	5	0.42
(1,3757)	2:1:B:MET:HE2	2:56:B:LEU:HD12	8	0.42
(1,3048)	2:42:C:ARG:HA	2:69:C:LEU:HD23	6	0.42
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	8	0.42
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD11	2	0.42
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD13	6	0.42
(1,1388)	1:599:A:ILE:HD11	1:562:A:TRP:HH2	3	0.42
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG23	6	0.41
(1,4014)	2:5:B:VAL:HG23	2:15:B:LEU:HG	6	0.41
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD12	6	0.41
(1,1773)	2:5:C:VAL:HA	2:66:C:THR:HG21	9	0.41
(1,1772)	2:5:C:VAL:HA	2:66:C:THR:HG21	9	0.41
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD11	1	0.41
(1,1534)	2:2:C:GLN:HE22	2:14:C:THR:HG22	6	0.41
(1,1510)	2:1:C:MET:HE2	2:67:C:LEU:HD11	10	0.41
(1,1491)	2:1:C:MET:HE3	2:56:C:LEU:HD12	5	0.41
(3,209)	2:27:B:LYS:HE2	2:69:B:LEU:HD11	6	0.4
(3,139)	2:66:C:THR:HG21	2:67:C:LEU:HD22	6	0.4
(1,5300)	2:41:B:GLN:HA	2:69:B:LEU:HD13	8	0.4
(1,5299)	2:41:B:GLN:HA	2:71:B:LEU:HD11	1	0.4
(1,5278)	2:40:B:GLN:HB2	2:71:B:LEU:HD12	1	0.4
(1,5107)	2:34:B:GLU:HG2	2:36:B:ILE:HG13	4	0.4
(1,5107)	2:34:B:GLU:HG3	2:36:B:ILE:HG13	6	0.4
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG23	6	0.4
(1,3697)	2:1:B:MET:HE2	2:3:B:ILE:HD11	4	0.4
(1,2843)	2:34:C:GLU:HG3	2:69:C:LEU:HD23	5	0.4
(1,2050)	2:15:C:LEU:HD23	2:29:C:LYS:HA	4	0.4
(1,1773)	2:5:C:VAL:HA	2:66:C:THR:HG21	6	0.4
(1,1772)	2:5:C:VAL:HA	2:66:C:THR:HG21	6	0.4
(1,1510)	2:1:C:MET:HE3	2:67:C:LEU:HD13	8	0.4
(1,1491)	2:1:C:MET:HE2	2:56:C:LEU:HD13	3	0.4
(1,505)	1:575:A:MET:HE1	1:575:A:MET:H	5	0.4
(1,505)	1:575:A:MET:HE2	1:575:A:MET:H	5	0.4
(1,505)	1:575:A:MET:HE3	1:575:A:MET:H	5	0.4
(1,5314)	2:42:B:ARG:HA	2:69:B:LEU:HD11	9	0.39
(1,5303)	2:41:B:GLN:HB3	2:69:B:LEU:HD12	5	0.39
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG21	2	0.39
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD12	5	0.39
(1,3799)	2:68:B:HIS:HA	2:5:B:VAL:HG11	2	0.39
(1,3697)	2:1:B:MET:HE2	2:3:B:ILE:HD11	9	0.39
(1,3014)	2:40:C:GLN:HB3	2:71:C:LEU:HD12	3	0.39
(1,2842)	2:34:C:GLU:HG3	2:69:C:LEU:HD13	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2071)	2:15:C:LEU:HD23	2:33:C:LYS:HD2	6	0.39
(1,1834)	2:6:C:LYS:HD2	2:66:C:THR:HG21	4	0.39
(1,1746)	2:5:C:VAL:HG21	2:15:C:LEU:HG	3	0.39
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD13	5	0.39
(1,1431)	2:1:C:MET:HE1	2:3:C:ILE:HD12	8	0.39
(1,1012)	1:543:A:THR:HB	1:573:A:LEU:HD23	7	0.39
(1,120)	1:503:A:ASP:H	1:506:A:LEU:H	4	0.39
(1,5282)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	7	0.38
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG21	2	0.38
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	6	0.38
(1,1995)	2:36:C:ILE:HG13	2:34:C:GLU:HG3	4	0.38
(1,1836)	2:6:C:LYS:HG2	2:66:C:THR:HG23	8	0.38
(1,1431)	2:1:C:MET:HE2	2:3:C:ILE:HD11	7	0.38
(1,5183)	2:36:B:ILE:HG23	2:71:B:LEU:HD13	1	0.37
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD21	5	0.37
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD12	1	0.37
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD11	2	0.37
(1,3697)	2:1:B:MET:HE3	2:3:B:ILE:HD11	10	0.37
(1,3013)	2:40:C:GLN:HB2	2:71:C:LEU:HD13	4	0.37
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	2	0.37
(1,1838)	2:6:C:LYS:HG3	2:66:C:THR:HG22	4	0.37
(1,1834)	2:6:C:LYS:HD2	2:66:C:THR:HG23	7	0.37
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD11	6	0.37
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD11	7	0.37
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD12	9	0.37
(1,1490)	2:1:C:MET:HE3	2:56:C:LEU:HD12	4	0.37
(1,5299)	2:41:B:GLN:HA	2:69:B:LEU:HD13	8	0.36
(1,5188)	2:36:B:ILE:HG21	2:71:B:LEU:HD12	7	0.36
(1,4104)	2:6:B:LYS:HG3	2:66:B:THR:HG23	6	0.36
(1,4031)	2:17:B:VAL:HG12	2:29:B:LYS:HG3	1	0.36
(1,4031)	2:17:B:VAL:HG12	2:29:B:LYS:HG2	10	0.36
(1,4012)	2:5:B:VAL:HG23	2:15:B:LEU:HG	1	0.36
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD11	8	0.36
(1,2071)	2:15:C:LEU:HD23	2:33:C:LYS:HD2	1	0.36
(1,2054)	2:15:C:LEU:HD22	2:29:C:LYS:HG2	5	0.36
(1,1835)	2:6:C:LYS:HE3	2:66:C:THR:HG21	5	0.36
(1,1620)	2:29:C:LYS:HA	2:33:C:LYS:HE2	10	0.36
(3,209)	2:27:B:LYS:HE2	2:69:B:LEU:HD11	8	0.35
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD11	4	0.35
(1,3776)	2:1:B:MET:HE3	2:67:B:LEU:HD11	10	0.35
(1,2071)	2:15:C:LEU:HD21	2:33:C:LYS:HD2	10	0.35
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD13	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:516:A:THR:HG21	2:72:C:ARG:HG2	4	0.35
(1,99)	1:516:A:THR:HG21	2:72:C:ARG:HG3	4	0.35
(1,99)	1:516:A:THR:HG22	2:72:C:ARG:HG2	4	0.35
(1,99)	1:516:A:THR:HG22	2:72:C:ARG:HG3	4	0.35
(1,99)	1:516:A:THR:HG23	2:72:C:ARG:HG2	4	0.35
(1,99)	1:516:A:THR:HG23	2:72:C:ARG:HG3	4	0.35
(3,209)	2:27:B:LYS:HE2	2:69:B:LEU:HD11	2	0.34
(1,4337)	2:15:B:LEU:HD11	2:33:B:LYS:HD2	4	0.34
(1,4031)	2:17:B:VAL:HG12	2:29:B:LYS:HG3	6	0.34
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD12	7	0.34
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD11	9	0.34
(1,2054)	2:15:C:LEU:HD23	2:29:C:LYS:HG2	10	0.34
(1,1837)	2:6:C:LYS:HG3	2:66:C:THR:HG22	5	0.34
(1,1586)	2:29:C:LYS:HA	2:15:C:LEU:HD22	5	0.34
(3,224)	2:36:B:ILE:HA	2:71:B:LEU:HD23	8	0.33
(3,34)	2:3:C:ILE:HG13	2:67:C:LEU:HB2	2	0.33
(3,26)	2:2:C:GLN:HG3	2:3:C:ILE:HA	10	0.33
(2,4)	1:484:A:LYS:O	1:488:A:ALA:N	5	0.33
(1,5300)	2:41:B:GLN:HA	2:71:B:LEU:HD11	2	0.33
(1,4320)	2:15:B:LEU:HD22	2:29:B:LYS:HG2	2	0.33
(1,4070)	2:6:B:LYS:HG2	2:10:B:GLY:HA2	3	0.33
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG23	9	0.33
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG23	9	0.33
(1,3697)	2:1:B:MET:HE3	2:3:B:ILE:HD12	7	0.33
(1,1881)	2:7:C:THR:HA	2:69:C:LEU:HD21	4	0.33
(1,1431)	2:1:C:MET:HE2	2:3:C:ILE:HD11	10	0.33
(1,254)	1:515:A:SER:HA	1:518:A:LEU:H	3	0.33
(1,120)	1:503:A:ASP:H	1:506:A:LEU:H	6	0.33
(3,153)	2:3:B:ILE:HG23	2:67:B:LEU:HG	4	0.32
(1,5283)	2:40:B:GLN:HB2	2:71:B:LEU:HD22	4	0.32
(1,5184)	2:36:B:ILE:HG22	2:71:B:LEU:HD23	8	0.32
(1,4102)	2:6:B:LYS:HG3	2:66:B:THR:HG23	5	0.32
(1,3886)	2:29:B:LYS:HA	2:33:B:LYS:HE2	1	0.32
(1,3697)	2:1:B:MET:HE1	2:3:B:ILE:HD11	8	0.32
(1,2050)	2:15:C:LEU:HD23	2:29:C:LYS:HA	10	0.32
(1,1835)	2:6:C:LYS:HE3	2:66:C:THR:HG21	2	0.32
(1,1533)	2:68:C:HIS:HA	2:5:C:VAL:HG12	1	0.32
(1,1533)	2:68:C:HIS:HA	2:5:C:VAL:HG12	9	0.32
(1,1510)	2:1:C:MET:HE1	2:67:C:LEU:HD11	6	0.32
(1,1431)	2:1:C:MET:HE1	2:3:C:ILE:HD13	2	0.32
(1,412)	1:547:A:MET:HE1	1:548:A:ASP:H	1	0.32
(1,412)	1:547:A:MET:HE2	1:548:A:ASP:H	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:547:A:MET:HE3	1:548:A:ASP:H	1	0.32
(3,146)	2:2:B:GLN:HG2	2:3:B:ILE:HA	5	0.31
(3,89)	2:27:C:LYS:HE2	2:69:C:LEU:HD12	10	0.31
(1,5316)	2:42:B:ARG:H	2:69:B:LEU:HD12	9	0.31
(1,4100)	2:6:B:LYS:HD2	2:66:B:THR:HG21	1	0.31
(1,3824)	2:3:B:ILE:HA	2:3:B:ILE:HD12	10	0.31
(1,3697)	2:1:B:MET:HE3	2:3:B:ILE:HD11	2	0.31
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD11	5	0.31
(1,1747)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	5	0.31
(1,505)	1:575:A:MET:HE1	1:575:A:MET:H	7	0.31
(1,505)	1:575:A:MET:HE2	1:575:A:MET:H	7	0.31
(1,505)	1:575:A:MET:HE3	1:575:A:MET:H	7	0.31
(3,26)	2:2:C:GLN:HG2	2:3:C:ILE:HA	5	0.3
(1,3697)	2:1:B:MET:HE3	2:3:B:ILE:HD11	3	0.3
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD11	10	0.3
(1,3014)	2:40:C:GLN:HB3	2:71:C:LEU:HD13	10	0.3
(1,2918)	2:36:C:ILE:HG23	2:71:C:LEU:HD21	3	0.3
(1,2843)	2:34:C:GLU:HG3	2:69:C:LEU:HD13	6	0.3
(1,1747)	2:5:C:VAL:HG22	2:13:C:ILE:HG13	6	0.3
(1,1747)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	10	0.3
(1,1620)	2:29:C:LYS:HA	2:33:C:LYS:HE2	2	0.3
(3,26)	2:2:C:GLN:HG2	2:3:C:ILE:HA	6	0.29
(2,3)	1:484:A:LYS:O	1:488:A:ALA:H	5	0.29
(1,4102)	2:6:B:LYS:HG3	2:66:B:THR:HG23	4	0.29
(1,3756)	2:1:B:MET:HE1	2:56:B:LEU:HD11	10	0.29
(1,3712)	2:1:B:MET:HE1	2:17:B:VAL:HB	6	0.29
(1,3041)	2:41:C:GLN:HG2	2:69:C:LEU:HD12	7	0.29
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD13	4	0.29
(1,2071)	2:15:C:LEU:HD21	2:33:C:LYS:HD2	4	0.29
(1,1939)	2:14:C:THR:HG21	2:15:C:LEU:H	8	0.29
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD12	10	0.29
(1,1450)	2:1:C:MET:HE1	2:17:C:VAL:HG22	8	0.29
(1,5299)	2:41:B:GLN:HA	2:71:B:LEU:HD11	2	0.28
(1,4260)	2:13:B:ILE:HG12	2:34:B:GLU:HG3	3	0.28
(1,4205)	2:14:B:THR:HG22	2:15:B:LEU:H	10	0.28
(1,3716)	2:1:B:MET:HE1	2:17:B:VAL:HG22	5	0.28
(1,3039)	2:41:C:GLN:HG2	2:69:C:LEU:HD12	7	0.28
(1,3012)	2:40:C:GLN:HB2	2:71:C:LEU:HD13	4	0.28
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	5	0.28
(1,1534)	2:2:C:GLN:HE22	2:14:C:THR:HG21	10	0.28
(1,1533)	2:68:C:HIS:HA	2:5:C:VAL:HG13	3	0.28
(1,1446)	2:1:C:MET:HE1	2:17:C:VAL:HB	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,26)	2:2:C:GLN:HG2	2:3:C:ILE:HA	3	0.27
(1,4102)	2:6:B:LYS:HG3	2:66:B:THR:HG23	10	0.27
(1,3798)	2:68:B:HIS:HA	2:5:B:VAL:HG11	9	0.27
(1,3757)	2:1:B:MET:HE1	2:56:B:LEU:HD13	5	0.27
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD23	6	0.27
(1,3033)	2:41:C:GLN:HA	2:69:C:LEU:HD11	5	0.27
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD11	1	0.27
(1,2918)	2:36:C:ILE:HG21	2:71:C:LEU:HD23	9	0.27
(1,1772)	2:5:C:VAL:HA	2:66:C:THR:HG23	8	0.27
(1,1558)	2:3:C:ILE:HA	2:3:C:ILE:HD13	8	0.27
(1,253)	1:515:A:SER:HA	1:517:A:ASP:H	8	0.27
(1,253)	1:515:A:SER:HA	1:517:A:ASP:H	10	0.27
(3,153)	2:3:B:ILE:HG22	2:67:B:LEU:HG	10	0.26
(2,4)	1:484:A:LYS:O	1:488:A:ALA:N	8	0.26
(1,4337)	2:15:B:LEU:HD23	2:33:B:LYS:HD2	3	0.26
(1,4102)	2:6:B:LYS:HG3	2:66:B:THR:HG23	2	0.26
(1,4012)	2:5:B:VAL:HG23	2:15:B:LEU:HG	6	0.26
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD23	8	0.26
(1,3716)	2:1:B:MET:HE1	2:17:B:VAL:HG21	6	0.26
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD11	3	0.26
(1,3043)	2:41:C:GLN:H	2:69:C:LEU:HD12	8	0.26
(1,1836)	2:6:C:LYS:HG3	2:66:C:THR:HG23	3	0.26
(1,1773)	2:5:C:VAL:HA	2:66:C:THR:HG23	8	0.26
(1,1620)	2:29:C:LYS:HA	2:33:C:LYS:HE2	7	0.26
(1,1446)	2:1:C:MET:HE2	2:17:C:VAL:HB	2	0.26
(3,26)	2:2:C:GLN:HG2	2:3:C:ILE:HA	4	0.25
(1,4316)	2:15:B:LEU:HD12	2:29:B:LYS:HA	2	0.25
(1,4103)	2:6:B:LYS:HG3	2:66:B:THR:HG21	8	0.25
(1,4102)	2:6:B:LYS:HG3	2:66:B:THR:HG21	7	0.25
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG22	10	0.25
(1,4014)	2:5:B:VAL:HG22	2:15:B:LEU:HG	2	0.25
(1,4014)	2:5:B:VAL:HG23	2:15:B:LEU:HG	5	0.25
(1,3886)	2:29:B:LYS:HA	2:33:B:LYS:HE3	7	0.25
(1,3756)	2:1:B:MET:HE1	2:56:B:LEU:HD13	7	0.25
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD12	2	0.25
(1,3033)	2:41:C:GLN:HA	2:69:C:LEU:HD13	4	0.25
(1,3015)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	8	0.25
(1,1533)	2:68:C:HIS:HA	2:5:C:VAL:HG12	5	0.25
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG22	7	0.24
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG22	10	0.24
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG22	7	0.24
(1,3992)	2:5:B:VAL:HG11	2:7:B:THR:HG21	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3776)	2:1:B:MET:HE2	2:67:B:LEU:HD13	4	0.24
(1,3756)	2:1:B:MET:HE2	2:56:B:LEU:HD12	8	0.24
(1,3738)	2:28:B:ALA:HB3	2:25:B:ASN:HA	8	0.24
(1,2917)	2:36:C:ILE:HG21	2:71:C:LEU:HD22	2	0.24
(1,1881)	2:7:C:THR:HA	2:69:C:LEU:HD23	10	0.24
(3,15)	1:518:A:LEU:CG	2:70:C:VAL:H	9	0.23
(1,4230)	2:13:B:ILE:HG23	2:15:B:LEU:HD12	1	0.23
(1,3823)	2:68:B:HIS:HA	2:66:B:THR:HG21	6	0.23
(1,3712)	2:1:B:MET:HE1	2:17:B:VAL:HB	10	0.23
(1,3033)	2:41:C:GLN:HA	2:69:C:LEU:HD23	6	0.23
(1,3017)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	3	0.23
(1,3011)	2:40:C:GLN:HB3	2:71:C:LEU:HD21	6	0.23
(1,2918)	2:36:C:ILE:HG21	2:71:C:LEU:HD11	1	0.23
(1,1838)	2:6:C:LYS:HG3	2:66:C:THR:HG22	5	0.23
(1,1765)	2:17:C:VAL:HG12	2:29:C:LYS:HG3	3	0.23
(1,1557)	2:68:C:HIS:HA	2:66:C:THR:HG22	9	0.23
(1,1490)	2:1:C:MET:HE3	2:56:C:LEU:HD12	5	0.23
(1,1468)	2:1:C:MET:HE1	2:19:C:PRO:HG2	1	0.23
(1,1468)	2:1:C:MET:HE1	2:19:C:PRO:HG3	1	0.23
(1,1468)	2:1:C:MET:HE2	2:19:C:PRO:HG2	1	0.23
(1,1468)	2:1:C:MET:HE2	2:19:C:PRO:HG3	1	0.23
(1,1468)	2:1:C:MET:HE3	2:19:C:PRO:HG2	1	0.23
(1,1468)	2:1:C:MET:HE3	2:19:C:PRO:HG3	1	0.23
(1,254)	1:515:A:SER:HA	1:518:A:LEU:H	7	0.23
(3,209)	2:27:B:LYS:HE2	2:69:B:LEU:HD11	1	0.22
(1,5307)	2:41:B:GLN:HG2	2:69:B:LEU:HD13	1	0.22
(1,4332)	2:36:B:ILE:HG13	2:30:B:ILE:HG23	3	0.22
(1,4204)	2:14:B:THR:HG23	2:14:B:THR:H	4	0.22
(1,4039)	2:5:B:VAL:HA	2:66:B:THR:HG22	1	0.22
(1,4038)	2:5:B:VAL:HA	2:66:B:THR:HG22	1	0.22
(1,1765)	2:17:C:VAL:HG12	2:29:C:LYS:HG3	1	0.22
(1,1764)	2:17:C:VAL:HG13	2:29:C:LYS:HG3	9	0.22
(1,1490)	2:1:C:MET:HE2	2:56:C:LEU:HD13	3	0.22
(1,1472)	2:28:C:ALA:HB1	2:25:C:ASN:HA	7	0.22
(1,1450)	2:1:C:MET:HE2	2:17:C:VAL:HG21	2	0.22
(3,146)	2:2:B:GLN:HG2	2:3:B:ILE:HA	6	0.21
(1,5305)	2:41:B:GLN:HG2	2:69:B:LEU:HD13	1	0.21
(1,4204)	2:14:B:THR:HG22	2:14:B:THR:H	10	0.21
(1,4102)	2:6:B:LYS:HG3	2:66:B:THR:HG21	1	0.21
(1,4031)	2:17:B:VAL:HG12	2:29:B:LYS:HG3	9	0.21
(1,3798)	2:68:B:HIS:HA	2:5:B:VAL:HG13	7	0.21
(1,3716)	2:1:B:MET:HE1	2:17:B:VAL:HG21	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3033)	2:41:C:GLN:HA	2:69:C:LEU:HD12	2	0.21
(1,3010)	2:40:C:GLN:HB3	2:71:C:LEU:HD21	7	0.21
(1,1881)	2:7:C:THR:HA	2:69:C:LEU:HD23	2	0.21
(1,1772)	2:5:C:VAL:HA	2:66:C:THR:HG22	5	0.21
(1,1747)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	2	0.21
(1,1533)	2:68:C:HIS:HA	2:5:C:VAL:HG12	2	0.21
(1,1491)	2:1:C:MET:HE1	2:56:C:LEU:HD12	1	0.21
(1,1450)	2:1:C:MET:HE3	2:17:C:VAL:HG21	9	0.21
(1,5180)	2:36:B:ILE:HD11	2:71:B:LEU:HD21	9	0.2
(1,4260)	2:13:B:ILE:HG12	2:34:B:GLU:HG3	4	0.2
(1,4030)	2:17:B:VAL:HG11	2:29:B:LYS:HG3	2	0.2
(1,3712)	2:1:B:MET:HE3	2:17:B:VAL:HB	2	0.2
(1,3017)	2:40:C:GLN:HB2	2:71:C:LEU:HD11	1	0.2
(1,1937)	2:12:C:THR:HG23	2:13:C:ILE:H	8	0.2
(1,1773)	2:5:C:VAL:HA	2:66:C:THR:HG22	5	0.2
(1,1620)	2:29:C:LYS:HA	2:33:C:LYS:HE2	1	0.2
(1,1446)	2:1:C:MET:HE3	2:17:C:VAL:HB	4	0.2
(1,100)	1:516:A:THR:HG21	2:72:C:ARG:HD2	5	0.2
(1,100)	1:516:A:THR:HG21	2:72:C:ARG:HD3	5	0.2
(1,100)	1:516:A:THR:HG22	2:72:C:ARG:HD2	5	0.2
(1,100)	1:516:A:THR:HG22	2:72:C:ARG:HD3	5	0.2
(1,100)	1:516:A:THR:HG23	2:72:C:ARG:HD2	5	0.2
(1,100)	1:516:A:THR:HG23	2:72:C:ARG:HD3	5	0.2
(3,146)	2:2:B:GLN:HG2	2:3:B:ILE:HA	9	0.19
(3,26)	2:2:C:GLN:HG2	2:3:C:ILE:HA	8	0.19
(1,4204)	2:14:B:THR:HG22	2:14:B:THR:H	5	0.19
(1,3738)	2:28:B:ALA:HB3	2:25:B:ASN:HA	5	0.19
(1,3716)	2:1:B:MET:HE3	2:17:B:VAL:HG21	2	0.19
(1,3642)	2:67:C:LEU:HB3	2:68:C:HIS:H	8	0.19
(1,3017)	2:40:C:GLN:HB2	2:71:C:LEU:HD21	10	0.19
(1,3015)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	2	0.19
(1,2918)	2:36:C:ILE:HG21	2:71:C:LEU:HD21	10	0.19
(3,224)	2:36:B:ILE:HA	2:71:B:LEU:HD22	7	0.18
(1,5908)	2:67:B:LEU:HB3	2:68:B:HIS:H	10	0.18
(1,5283)	2:40:B:GLN:HB2	2:71:B:LEU:HD23	6	0.18
(1,4337)	2:15:B:LEU:HD21	2:33:B:LYS:HD2	8	0.18
(1,4205)	2:14:B:THR:HG23	2:15:B:LEU:H	4	0.18
(1,3992)	2:5:B:VAL:HG13	2:7:B:THR:HG22	3	0.18
(1,3886)	2:29:B:LYS:HA	2:33:B:LYS:HE2	2	0.18
(1,3775)	2:1:B:MET:HG3	2:63:B:LYS:HA	6	0.18
(1,3738)	2:28:B:ALA:HB2	2:25:B:ASN:HA	7	0.18
(1,3738)	2:28:B:ALA:HB2	2:25:B:ASN:HA	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3712)	2:1:B:MET:HE1	2:17:B:VAL:HB	7	0.18
(1,2227)	2:20:C:SER:HB3	2:21:C:ASP:H	2	0.18
(1,1836)	2:6:C:LYS:HG3	2:66:C:THR:HG23	7	0.18
(1,1509)	2:1:C:MET:HG3	2:63:C:LYS:HA	4	0.18
(1,1450)	2:1:C:MET:HE3	2:17:C:VAL:HG21	4	0.18
(3,24)	2:1:C:MET:HE1	2:67:C:LEU:HD12	3	0.17
(1,5908)	2:67:B:LEU:HB3	2:68:B:HIS:H	4	0.17
(1,5276)	2:40:B:GLN:HB3	2:71:B:LEU:HD23	7	0.17
(1,4146)	2:7:B:THR:HA	2:69:B:LEU:HD23	2	0.17
(1,3993)	2:5:B:VAL:HG11	2:7:B:THR:HG21	7	0.17
(1,3738)	2:28:B:ALA:HB1	2:25:B:ASN:HA	2	0.17
(1,3716)	2:1:B:MET:HE3	2:17:B:VAL:HG22	4	0.17
(1,3716)	2:1:B:MET:HE1	2:17:B:VAL:HG23	7	0.17
(1,3697)	2:1:B:MET:HE3	2:3:B:ILE:HD12	1	0.17
(1,3017)	2:40:C:GLN:HB2	2:71:C:LEU:HD22	8	0.17
(1,1837)	2:6:C:LYS:HG3	2:66:C:THR:HG21	2	0.17
(1,1765)	2:17:C:VAL:HG11	2:29:C:LYS:HG3	4	0.17
(1,1620)	2:29:C:LYS:HA	2:33:C:LYS:HE2	4	0.17
(1,1509)	2:1:C:MET:HG3	2:63:C:LYS:HA	9	0.17
(1,253)	1:515:A:SER:HA	1:517:A:ASP:H	9	0.17
(3,33)	2:3:C:ILE:HG21	2:67:C:LEU:HG	1	0.16
(1,5300)	2:41:B:GLN:HA	2:69:B:LEU:HD12	3	0.16
(1,5184)	2:36:B:ILE:HG22	2:71:B:LEU:HD11	2	0.16
(1,5180)	2:36:B:ILE:HD13	2:71:B:LEU:HD23	5	0.16
(1,4261)	2:13:B:ILE:HG12	2:34:B:GLU:HG3	3	0.16
(1,4158)	2:7:B:THR:HG23	2:69:B:LEU:HD22	10	0.16
(1,3757)	2:1:B:MET:HE1	2:56:B:LEU:HD13	1	0.16
(1,1938)	2:14:C:THR:HG23	2:14:C:THR:H	6	0.16
(1,1938)	2:14:C:THR:HG22	2:14:C:THR:H	7	0.16
(1,1938)	2:14:C:THR:HG22	2:14:C:THR:H	8	0.16
(1,1837)	2:6:C:LYS:HG3	2:66:C:THR:HG21	9	0.16
(1,1749)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	5	0.16
(1,1749)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	10	0.16
(1,1450)	2:1:C:MET:HE3	2:17:C:VAL:HG21	10	0.16
(1,412)	1:547:A:MET:HE1	1:548:A:ASP:H	7	0.16
(1,412)	1:547:A:MET:HE2	1:548:A:ASP:H	7	0.16
(1,412)	1:547:A:MET:HE3	1:548:A:ASP:H	7	0.16
(1,120)	1:503:A:ASP:H	1:506:A:LEU:H	8	0.16
(3,33)	2:3:C:ILE:HG21	2:67:C:LEU:HG	3	0.15
(2,3)	1:484:A:LYS:O	1:488:A:ALA:H	8	0.15
(1,4316)	2:15:B:LEU:HD22	2:29:B:LYS:HA	3	0.15
(1,4260)	2:13:B:ILE:HG12	2:34:B:GLU:HG3	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4204)	2:14:B:THR:HG23	2:14:B:THR:H	6	0.15
(1,4204)	2:14:B:THR:HG23	2:14:B:THR:H	7	0.15
(1,4204)	2:14:B:THR:HG22	2:14:B:THR:H	8	0.15
(1,3852)	2:29:B:LYS:HA	2:15:B:LEU:HD13	9	0.15
(1,3738)	2:28:B:ALA:HB3	2:25:B:ASN:HA	1	0.15
(1,3642)	2:67:C:LEU:HB3	2:68:C:HIS:H	6	0.15
(1,3017)	2:40:C:GLN:HB2	2:71:C:LEU:HD22	2	0.15
(1,2054)	2:15:C:LEU:HD21	2:29:C:LYS:HG2	7	0.15
(1,2050)	2:15:C:LEU:HD22	2:29:C:LYS:HA	1	0.15
(1,1887)	2:7:C:THR:HB	2:69:C:LEU:HD21	3	0.15
(1,1749)	2:5:C:VAL:HG22	2:13:C:ILE:HG13	6	0.15
(1,1557)	2:68:C:HIS:HA	2:66:C:THR:HG23	2	0.15
(1,1450)	2:1:C:MET:HE3	2:17:C:VAL:HG21	7	0.15
(1,1431)	2:1:C:MET:HE1	2:3:C:ILE:HD13	3	0.15
(3,146)	2:2:B:GLN:HG2	2:3:B:ILE:HA	8	0.14
(1,5898)	2:70:B:VAL:HG11	2:68:B:HIS:HB3	3	0.14
(1,5898)	2:70:B:VAL:HG12	2:68:B:HIS:HB3	8	0.14
(1,5364)	2:69:B:LEU:HD11	2:70:B:VAL:H	9	0.14
(1,5279)	2:40:B:GLN:HB2	2:71:B:LEU:HD21	10	0.14
(1,4320)	2:15:B:LEU:HD13	2:29:B:LYS:HG3	1	0.14
(1,4320)	2:15:B:LEU:HD23	2:29:B:LYS:HG2	8	0.14
(1,4204)	2:14:B:THR:HG21	2:14:B:THR:H	2	0.14
(1,4104)	2:6:B:LYS:HG3	2:66:B:THR:HG21	8	0.14
(1,4095)	2:6:B:LYS:HB2	2:66:B:THR:HG21	9	0.14
(1,4013)	2:5:B:VAL:HG23	2:13:B:ILE:HG13	9	0.14
(1,3712)	2:1:B:MET:HE2	2:17:B:VAL:HB	8	0.14
(1,2842)	2:34:C:GLU:HG3	2:69:C:LEU:HD23	2	0.14
(1,2841)	2:34:C:GLU:HG3	2:36:C:ILE:HG13	4	0.14
(1,2601)	2:27:C:LYS:HB3	2:38:C:PRO:HG3	8	0.14
(1,1938)	2:14:C:THR:HG23	2:14:C:THR:H	3	0.14
(1,1938)	2:14:C:THR:HG22	2:14:C:THR:H	10	0.14
(1,1881)	2:7:C:THR:HA	2:69:C:LEU:HD23	5	0.14
(1,1834)	2:6:C:LYS:HD2	2:66:C:THR:HG21	5	0.14
(1,1780)	2:5:C:VAL:HG12	2:67:C:LEU:HB2	9	0.14
(1,1747)	2:5:C:VAL:HG23	2:13:C:ILE:HG13	1	0.14
(1,1509)	2:1:C:MET:HG3	2:63:C:LYS:HA	3	0.14
(1,1472)	2:28:C:ALA:HB3	2:25:C:ASN:HA	3	0.14
(1,1446)	2:1:C:MET:HE3	2:17:C:VAL:HB	10	0.14
(3,52)	2:34:C:GLU:HG3	2:30:C:ILE:HD11	5	0.13
(1,4283)	2:15:B:LEU:HA	2:15:B:LEU:HD13	7	0.13
(1,4204)	2:14:B:THR:HG21	2:14:B:THR:H	1	0.13
(1,4100)	2:6:B:LYS:HD2	2:66:B:THR:HG22	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4030)	2:17:B:VAL:HG11	2:29:B:LYS:HG3	5	0.13
(1,3798)	2:68:B:HIS:HA	2:5:B:VAL:HG13	8	0.13
(1,3716)	2:1:B:MET:HE2	2:17:B:VAL:HG21	8	0.13
(1,3716)	2:1:B:MET:HE3	2:17:B:VAL:HG21	9	0.13
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD22	9	0.13
(1,2842)	2:34:C:GLU:HG3	2:69:C:LEU:HD21	3	0.13
(1,2050)	2:15:C:LEU:HD21	2:29:C:LYS:HA	7	0.13
(1,1938)	2:14:C:THR:HG23	2:14:C:THR:H	5	0.13
(1,1726)	2:5:C:VAL:HG12	2:7:C:THR:HG23	6	0.13
(1,1468)	2:1:C:MET:HE1	2:19:C:PRO:HG2	5	0.13
(1,1468)	2:1:C:MET:HE1	2:19:C:PRO:HG3	5	0.13
(1,1468)	2:1:C:MET:HE2	2:19:C:PRO:HG2	5	0.13
(1,1468)	2:1:C:MET:HE2	2:19:C:PRO:HG3	5	0.13
(1,1468)	2:1:C:MET:HE3	2:19:C:PRO:HG2	5	0.13
(1,1468)	2:1:C:MET:HE3	2:19:C:PRO:HG3	5	0.13
(1,5908)	2:67:B:LEU:HB3	2:68:B:HIS:H	5	0.12
(1,5299)	2:41:B:GLN:HA	2:69:B:LEU:HD12	3	0.12
(1,5184)	2:36:B:ILE:HG22	2:71:B:LEU:HD23	5	0.12
(1,4867)	2:27:B:LYS:HB3	2:38:B:PRO:HG3	7	0.12
(1,4337)	2:15:B:LEU:HD13	2:33:B:LYS:HD2	10	0.12
(1,4204)	2:14:B:THR:HG22	2:14:B:THR:H	9	0.12
(1,3993)	2:5:B:VAL:HG13	2:7:B:THR:HG22	3	0.12
(1,3800)	2:2:B:GLN:HE22	2:14:B:THR:HG23	2	0.12
(1,3798)	2:68:B:HIS:HA	2:5:B:VAL:HG12	5	0.12
(1,3775)	2:1:B:MET:HG3	2:63:B:LYS:HA	5	0.12
(1,3697)	2:1:B:MET:HE3	2:3:B:ILE:HD12	5	0.12
(1,3642)	2:67:C:LEU:HB3	2:68:C:HIS:H	3	0.12
(1,1938)	2:14:C:THR:HG22	2:14:C:THR:H	4	0.12
(1,1887)	2:7:C:THR:HB	2:71:C:LEU:HD13	2	0.12
(1,1887)	2:7:C:THR:HB	2:69:C:LEU:HD23	10	0.12
(1,1765)	2:17:C:VAL:HG13	2:29:C:LYS:HG3	7	0.12
(1,1469)	2:1:C:MET:HE2	2:19:C:PRO:HG3	1	0.12
(1,1450)	2:1:C:MET:HE2	2:17:C:VAL:HG21	3	0.12
(1,1450)	2:1:C:MET:HE3	2:17:C:VAL:HG23	5	0.12
(1,1446)	2:1:C:MET:HE3	2:17:C:VAL:HB	7	0.12
(1,253)	1:515:A:SER:HA	1:517:A:ASP:H	2	0.12
(3,209)	2:27:B:LYS:HE2	2:69:B:LEU:HD12	9	0.11
(3,24)	2:1:C:MET:HE2	2:67:C:LEU:HD11	9	0.11
(1,5300)	2:41:B:GLN:HA	2:69:B:LEU:HD11	7	0.11
(1,5300)	2:41:B:GLN:HA	2:71:B:LEU:HD13	9	0.11
(1,5140)	2:36:B:ILE:HG21	2:37:B:PRO:HB2	10	0.11
(1,4513)	2:52:B:ASP:HB2	2:24:B:GLU:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4205)	2:14:B:THR:HG22	2:15:B:LEU:H	7	0.11
(1,4100)	2:6:B:LYS:HD2	2:66:B:THR:HG21	7	0.11
(1,3886)	2:29:B:LYS:HA	2:33:B:LYS:HE2	10	0.11
(1,3800)	2:2:B:GLN:HE22	2:14:B:THR:HG21	9	0.11
(1,3775)	2:1:B:MET:HG3	2:63:B:LYS:HA	1	0.11
(1,3716)	2:1:B:MET:HE1	2:17:B:VAL:HG23	3	0.11
(1,3712)	2:1:B:MET:HE3	2:17:B:VAL:HB	4	0.11
(1,3712)	2:1:B:MET:HE3	2:17:B:VAL:HB	9	0.11
(1,3034)	2:41:C:GLN:HA	2:69:C:LEU:HD22	1	0.11
(1,2247)	2:52:C:ASP:HB2	2:24:C:GLU:HB2	1	0.11
(1,2247)	2:52:C:ASP:HB2	2:24:C:GLU:HB2	6	0.11
(1,2247)	2:52:C:ASP:HB2	2:24:C:GLU:HB2	10	0.11
(1,2066)	2:36:C:ILE:HG13	2:30:C:ILE:HG23	7	0.11
(1,1938)	2:14:C:THR:HG23	2:14:C:THR:H	1	0.11
(1,1938)	2:14:C:THR:HG21	2:14:C:THR:H	2	0.11
(1,1938)	2:14:C:THR:HG22	2:14:C:THR:H	9	0.11
(1,1557)	2:68:C:HIS:HA	2:66:C:THR:HG23	5	0.11
(3,144)	2:1:B:MET:HE3	2:67:B:LEU:HD13	1	0.1
(1,4513)	2:52:B:ASP:HB2	2:24:B:GLU:HB2	7	0.1
(1,4320)	2:15:B:LEU:HD22	2:29:B:LYS:HG2	6	0.1
(1,3015)	2:40:C:GLN:HB3	2:71:C:LEU:HD22	5	0.1
(1,2050)	2:15:C:LEU:HD21	2:29:C:LYS:HA	3	0.1
(1,1472)	2:28:C:ALA:HB2	2:25:C:ASN:HA	8	0.1
(1,472)	1:556:A:ILE:HG21	1:554:A:THR:H	5	0.1
(1,472)	1:556:A:ILE:HG22	1:554:A:THR:H	5	0.1
(1,472)	1:556:A:ILE:HG23	1:554:A:THR:H	5	0.1
(1,120)	1:503:A:ASP:H	1:506:A:LEU:H	3	0.1

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

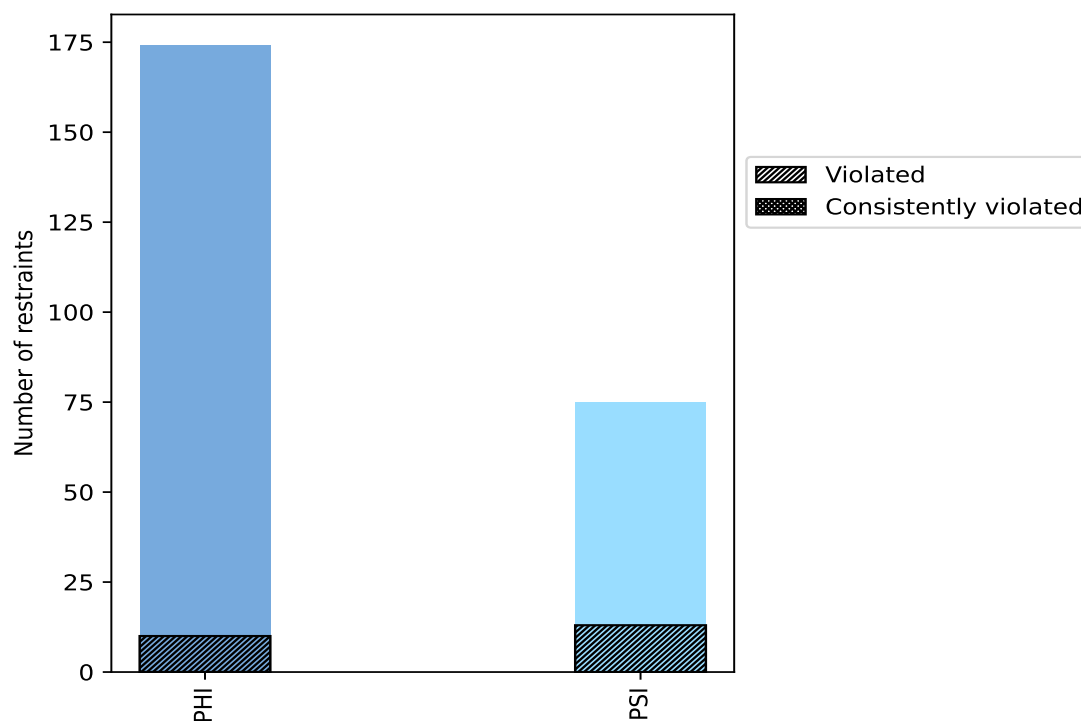
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	174	69.9	10	5.7	4.0	0	0.0	0.0
PSI	75	30.1	13	17.3	5.2	0	0.0	0.0
Total	249	100.0	23	9.2	9.2	0	0.0	0.0

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

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



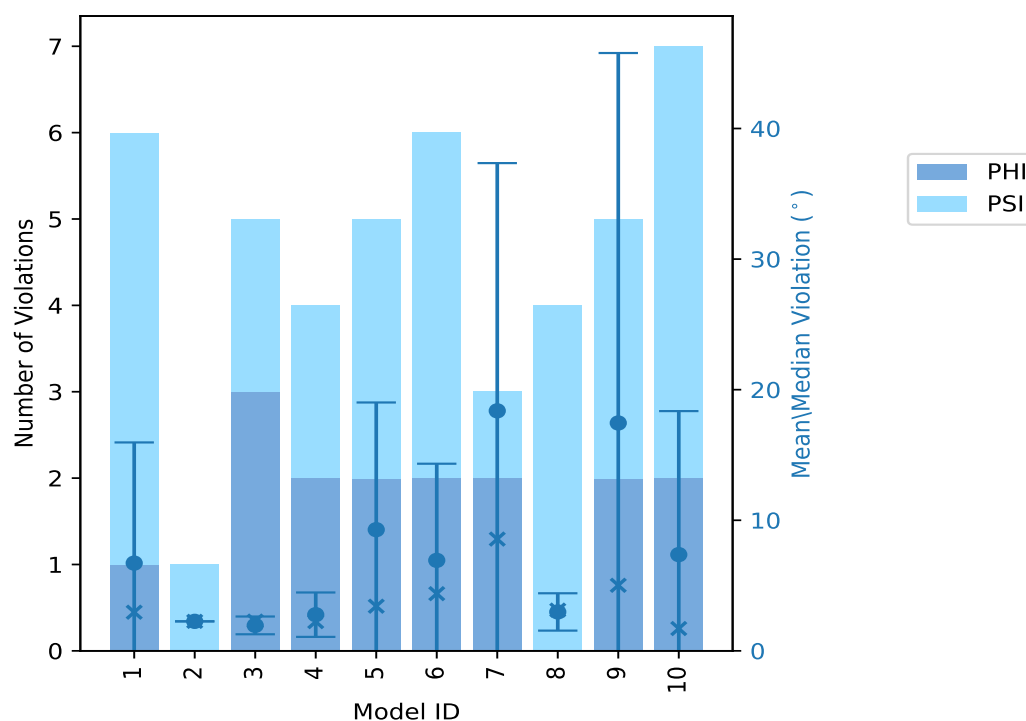
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	1	5	6	6.72	27.21	9.24	2.96
2	0	1	1	2.26	2.26	0.0	2.26
3	3	2	5	1.95	2.83	0.68	2.28
4	2	2	4	2.77	5.55	1.7	2.24
5	2	3	5	9.28	26.01	9.74	3.42
6	2	4	6	6.93	23.11	7.4	4.38
7	2	1	3	18.38	44.92	18.97	8.56
8	0	4	4	2.98	4.58	1.43	3.12
9	2	3	5	17.45	74.03	28.33	5.02
10	2	5	7	7.37	33.73	10.99	1.71

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



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

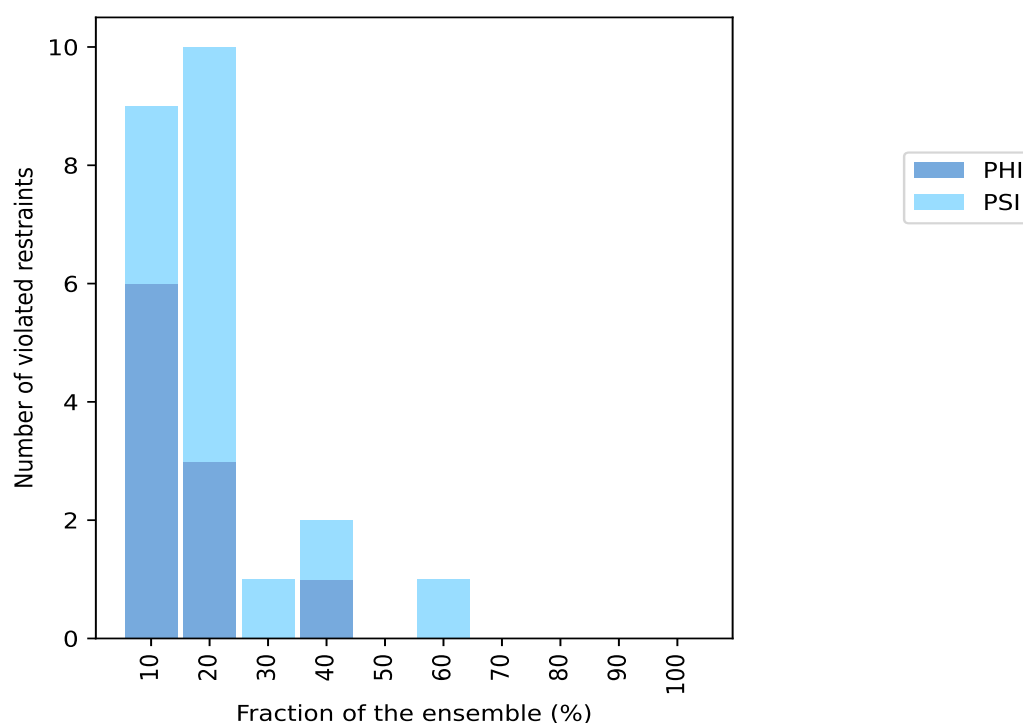
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
6	3	9	1	10.0
3	7	10	2	20.0
0	1	1	3	30.0
1	1	2	4	40.0
0	0	0	5	50.0
0	1	1	6	60.0
0	0	0	7	70.0
0	0	0	8	80.0
0	0	0	9	90.0
0	0	0	10	100.0

¹ Number of models with violations

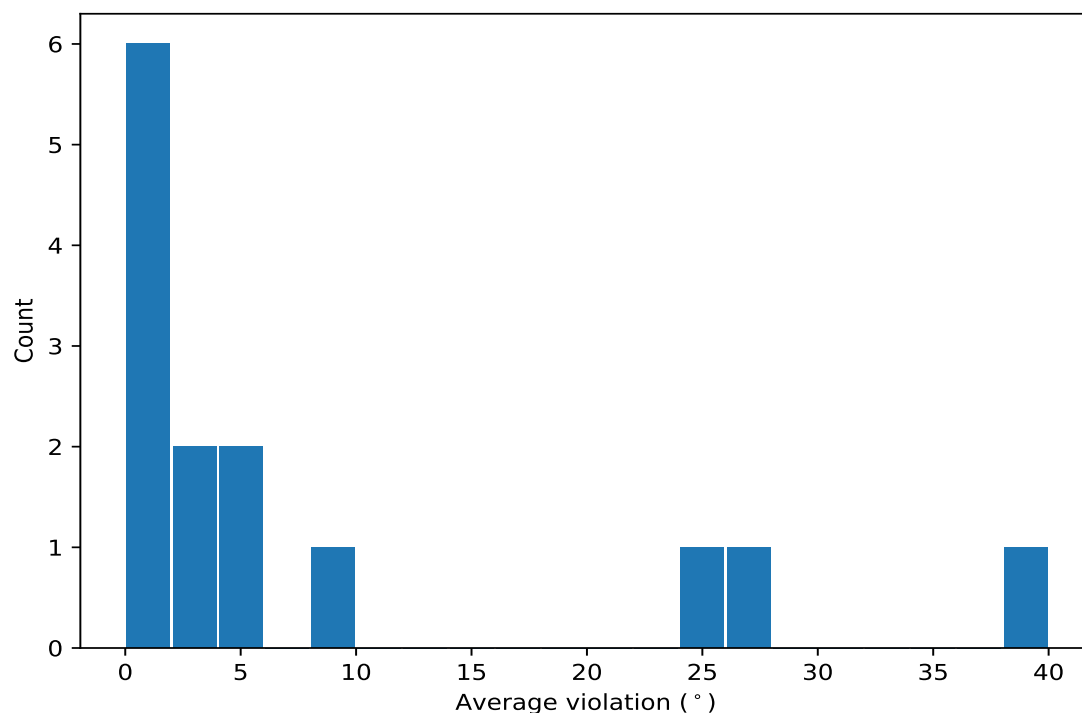
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,35)	1:513:A:ALA:N	1:513:A:ALA:CA	1:513:A:ALA:C	1:514:A:ALA:N	6	4.18	1.24	3.96
(1,14)	1:502:A:ASN:C	1:503:A:ASP:N	1:503:A:ASP:CA	1:503:A:ASP:C	4	26.82	28.79	15.78
(1,92)	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	1:553:A:ARG:N	4	8.15	4.08	6.92
(1,111)	1:571:A:GLY:N	1:571:A:GLY:CA	1:571:A:GLY:C	1:572:A:ILE:N	3	1.82	0.31	1.6
(1,208)	2:7:B:THR:C	2:8:B:LEU:N	2:8:B:LEU:CA	2:8:B:LEU:C	2	39.33	5.6	39.33
(1,117)	1:578:A:GLY:C	1:579:A:GLU:N	1:579:A:GLU:CA	1:579:A:GLU:C	2	25.16	2.05	25.16
(1,118)	1:579:A:GLU:N	1:579:A:GLU:CA	1:579:A:GLU:C	1:580:A:GLN:N	2	4.83	1.14	4.83
(1,141)	1:596:A:THR:N	1:596:A:THR:CA	1:596:A:THR:C	1:597:A:SER:N	2	3.72	2.56	3.72
(1,12)	1:498:A:ALA:N	1:498:A:ALA:CA	1:498:A:ALA:C	1:499:A:GLY:N	2	3.1	1.96	3.1
(1,97)	1:564:A:ARG:N	1:564:A:ARG:CA	1:564:A:ARG:C	1:565:A:PHE:N	2	1.86	0.15	1.86
(1,66)	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	1:538:A:CYS:N	2	1.78	0.56	1.78
(1,200)	2:67:C:LEU:C	2:68:C:HIS:N	2:68:C:HIS:CA	2:68:C:HIS:C	2	1.69	0.49	1.69
(1,155)	1:606:A:CYS:N	1:606:A:CYS:CA	1:606:A:CYS:C	1:607:A:ALA:N	2	1.68	0.42	1.68

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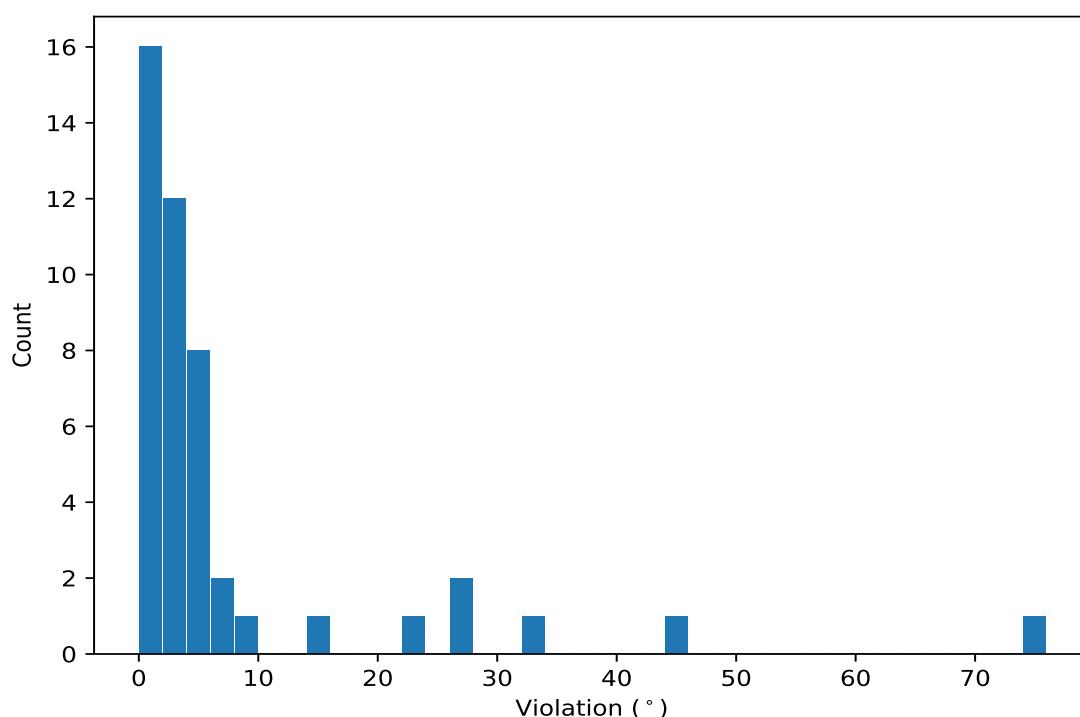
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,38)	1:519:A:PRO:N	1:519:A:PRO:CA	1:519:A:PRO:C	1:520:A:ILE:N	2	1.1	0.01	1.1

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

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

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

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,14)	1:502:A:ASN:C	1:503:A:ASP:N	1:503:A:ASP:CA	1:503:A:ASP:C	9	74.03
(1,208)	2:7:B:THR:C	2:8:B:LEU:N	2:8:B:LEU:CA	2:8:B:LEU:C	7	44.92
(1,208)	2:7:B:THR:C	2:8:B:LEU:N	2:8:B:LEU:CA	2:8:B:LEU:C	10	33.73
(1,117)	1:578:A:GLY:C	1:579:A:GLU:N	1:579:A:GLU:CA	1:579:A:GLU:C	1	27.21
(1,14)	1:502:A:ASN:C	1:503:A:ASP:N	1:503:A:ASP:CA	1:503:A:ASP:C	5	26.01
(1,117)	1:578:A:GLY:C	1:579:A:GLU:N	1:579:A:GLU:CA	1:579:A:GLU:C	6	23.11

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,92)	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	1:553:A:ARG:N	5	14.63
(1,92)	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	1:553:A:ARG:N	7	8.56
(1,35)	1:513:A:ALA:N	1:513:A:ALA:CA	1:513:A:ALA:C	1:514:A:ALA:N	10	6.52
(1,141)	1:596:A:THR:N	1:596:A:THR:CA	1:596:A:THR:C	1:597:A:SER:N	10	6.28
(1,118)	1:579:A:GLU:N	1:579:A:GLU:CA	1:579:A:GLU:C	1:580:A:GLN:N	6	5.97
(1,14)	1:502:A:ASN:C	1:503:A:ASP:N	1:503:A:ASP:CA	1:503:A:ASP:C	4	5.55
(1,92)	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	1:553:A:ARG:N	6	5.28
(1,12)	1:498:A:ALA:N	1:498:A:ALA:CA	1:498:A:ALA:C	1:499:A:GLY:N	9	5.05
(1,13)	1:498:A:ALA:C	1:499:A:GLY:N	1:499:A:GLY:CA	1:499:A:GLY:C	9	5.02
(1,35)	1:513:A:ALA:N	1:513:A:ALA:CA	1:513:A:ALA:C	1:514:A:ALA:N	8	4.58
(1,35)	1:513:A:ALA:N	1:513:A:ALA:CA	1:513:A:ALA:C	1:514:A:ALA:N	1	4.44
(1,92)	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	1:553:A:ARG:N	8	4.14
(1,118)	1:579:A:GLU:N	1:579:A:GLU:CA	1:579:A:GLU:C	1:580:A:GLN:N	1	3.69
(1,35)	1:513:A:ALA:N	1:513:A:ALA:CA	1:513:A:ALA:C	1:514:A:ALA:N	6	3.47
(1,35)	1:513:A:ALA:N	1:513:A:ALA:CA	1:513:A:ALA:C	1:514:A:ALA:N	5	3.42
(1,156)	2:2:C:GLN:C	2:3:C:ILE:N	2:3:C:ILE:CA	2:3:C:ILE:C	3	2.83
(1,35)	1:513:A:ALA:N	1:513:A:ALA:CA	1:513:A:ALA:C	1:514:A:ALA:N	4	2.63
(1,66)	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	1:538:A:CYS:N	3	2.34
(1,64)	1:535:A:VAL:N	1:535:A:VAL:CA	1:535:A:VAL:C	1:536:A:GLY:N	3	2.28
(1,111)	1:571:A:GLY:N	1:571:A:GLY:CA	1:571:A:GLY:C	1:572:A:ILE:N	2	2.26
(1,8)	1:496:A:ALA:N	1:496:A:ALA:CA	1:496:A:ALA:C	1:497:A:PHE:N	1	2.23
(1,200)	2:67:C:LEU:C	2:68:C:HIS:N	2:68:C:HIS:CA	2:68:C:HIS:C	6	2.18
(1,155)	1:606:A:CYS:N	1:606:A:CYS:CA	1:606:A:CYS:C	1:607:A:ALA:N	8	2.11
(1,97)	1:564:A:ARG:N	1:564:A:ARG:CA	1:564:A:ARG:C	1:565:A:PHE:N	9	2.0
(1,211)	2:13:B:ILE:C	2:14:B:THR:N	2:14:B:THR:CA	2:14:B:THR:C	4	1.84
(1,97)	1:564:A:ARG:N	1:564:A:ARG:CA	1:564:A:ARG:C	1:565:A:PHE:N	10	1.71
(1,14)	1:502:A:ASN:C	1:503:A:ASP:N	1:503:A:ASP:CA	1:503:A:ASP:C	7	1.67
(1,111)	1:571:A:GLY:N	1:571:A:GLY:CA	1:571:A:GLY:C	1:572:A:ILE:N	1	1.6
(1,111)	1:571:A:GLY:N	1:571:A:GLY:CA	1:571:A:GLY:C	1:572:A:ILE:N	6	1.59
(1,155)	1:606:A:CYS:N	1:606:A:CYS:CA	1:606:A:CYS:C	1:607:A:ALA:N	5	1.26
(1,66)	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	1:538:A:CYS:N	10	1.21
(1,200)	2:67:C:LEU:C	2:68:C:HIS:N	2:68:C:HIS:CA	2:68:C:HIS:C	3	1.2
(1,141)	1:596:A:THR:N	1:596:A:THR:CA	1:596:A:THR:C	1:597:A:SER:N	9	1.17
(1,12)	1:498:A:ALA:N	1:498:A:ALA:CA	1:498:A:ALA:C	1:499:A:GLY:N	1	1.14
(1,203)	2:2:B:GLN:C	2:3:B:ILE:N	2:3:B:ILE:CA	2:3:B:ILE:C	5	1.1
(1,67)	1:539:A:ASN:C	1:540:A:GLY:N	1:540:A:GLY:CA	1:540:A:GLY:C	3	1.1
(1,38)	1:519:A:PRO:N	1:519:A:PRO:CA	1:519:A:PRO:C	1:520:A:ILE:N	8	1.1
(1,38)	1:519:A:PRO:N	1:519:A:PRO:CA	1:519:A:PRO:C	1:520:A:ILE:N	10	1.09
(1,34)	1:512:A:ILE:C	1:513:A:ALA:N	1:513:A:ALA:CA	1:513:A:ALA:C	10	1.07
(1,4)	1:489:A:ALA:N	1:489:A:ALA:CA	1:489:A:ALA:C	1:490:A:ILE:N	4	1.05