



Full wwPDB NMR Structure Validation Report ⓘ

Sep 9, 2026 – 10:18 AM JST

PDB ID : 9WKT / pdb_00009wkt
BMRB ID : 36783
Title : mature Mba1, UniProt P38300, residues 34-278, *Saccharomyces cerevisiae*
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Deposited on : 2025-09-01

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 : v1.2.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

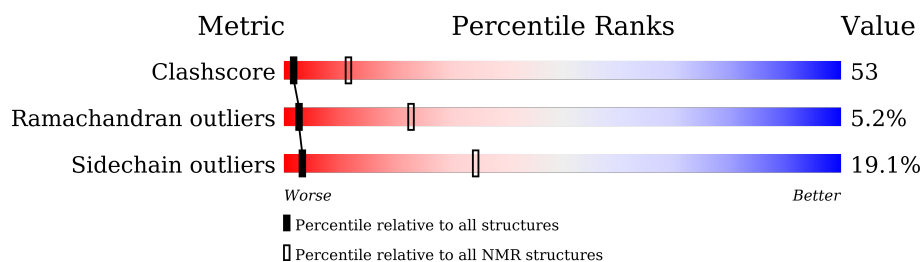
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	210	

2 Ensemble composition and analysis

This entry contains 15 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:78-A:103, A:116-A:177, A:190-A:208, A:213-A:231, A:235-A:243 (135)	1.40	3

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3435 atoms, of which 1746 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Inner membrane mitoribosome receptor MBA1, mitochondrial.

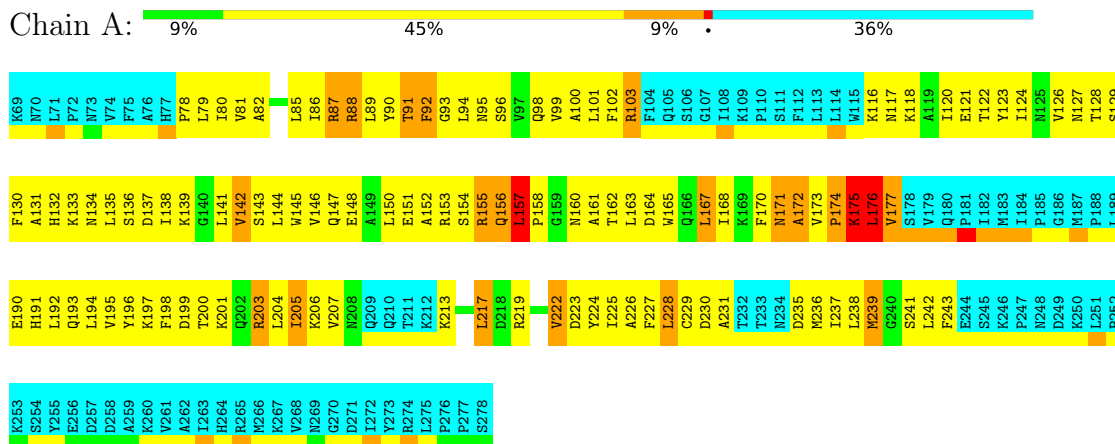
Mol	Chain	Residues	Atoms						Trace
1	A	210	Total	C	H	N	O	S	0
			3435	1092	1746	290	301	6	

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: Inner membrane mitoribosome receptor MBA1, mitochondrial

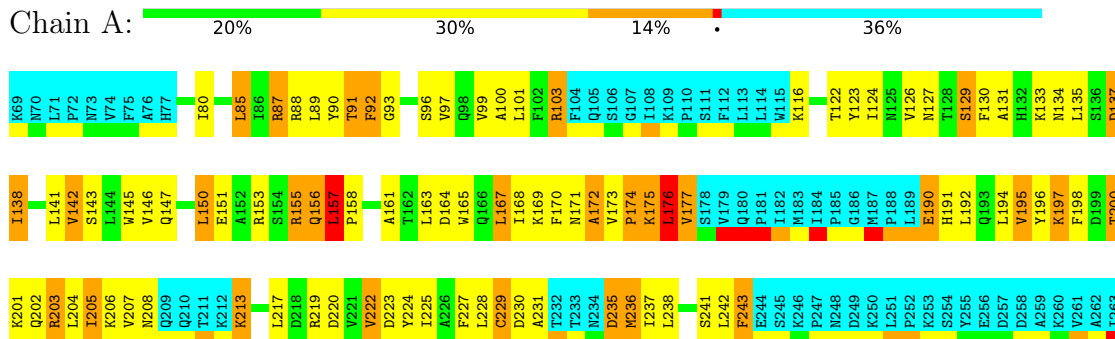


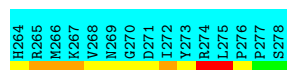
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

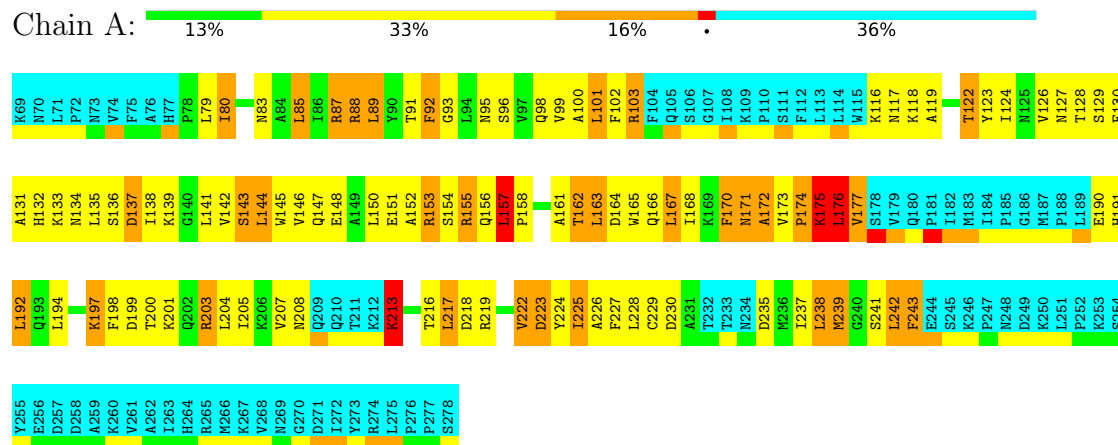
- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial





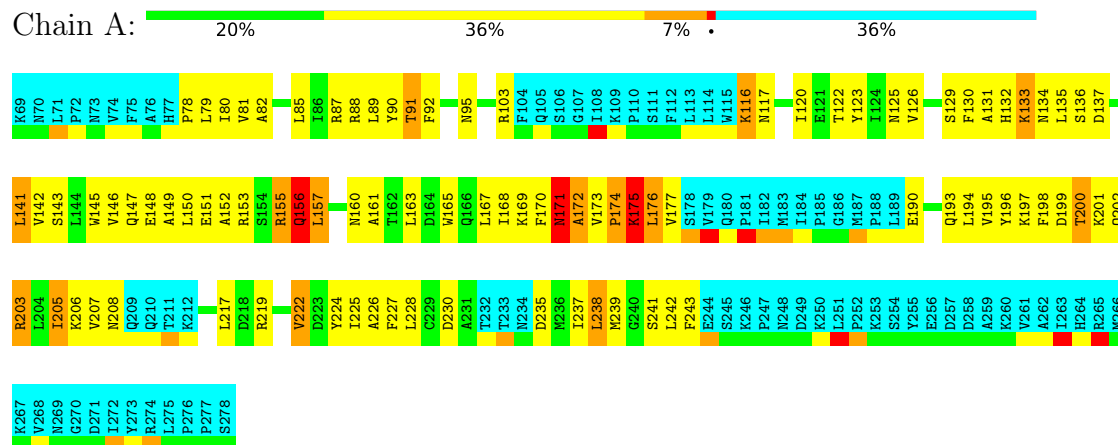
4.2.2 Score per residue for model 2

- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



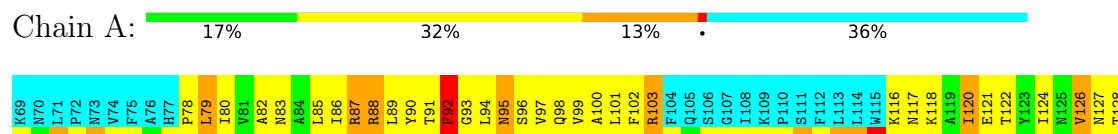
4.2.3 Score per residue for model 3 (medoid)

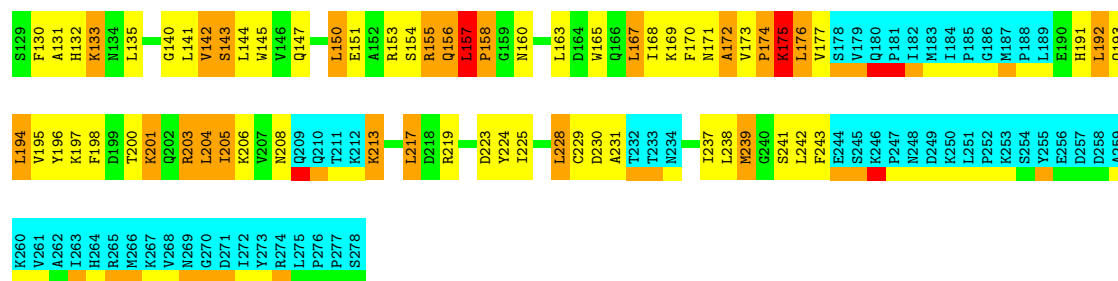
- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



4.2.4 Score per residue for model 4

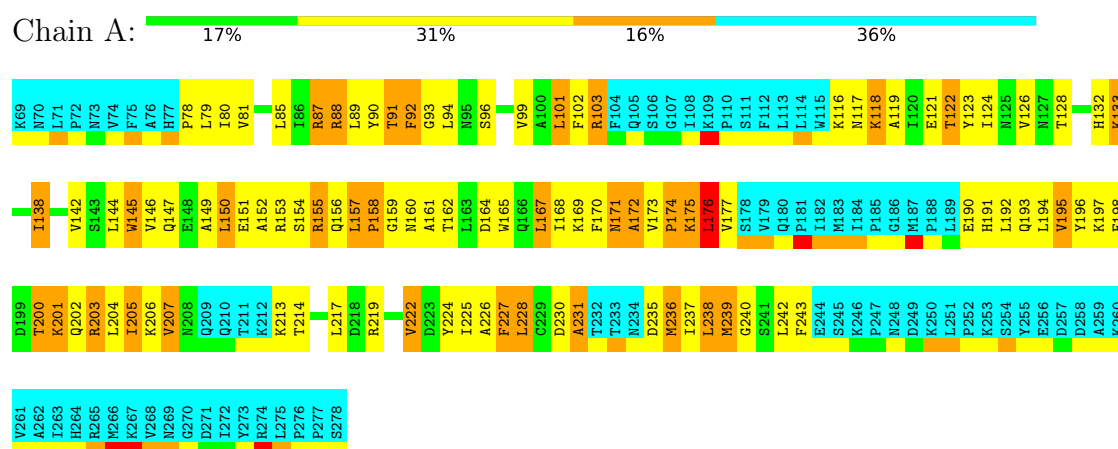
- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial





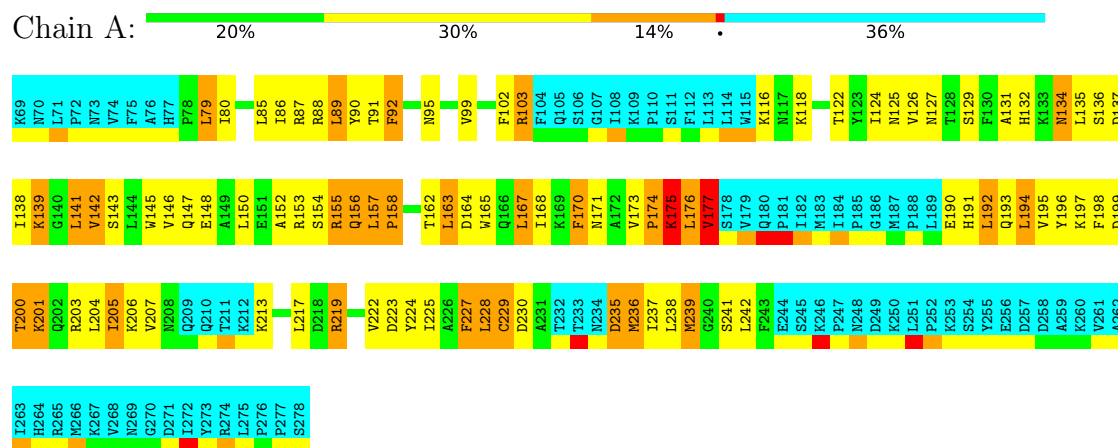
4.2.5 Score per residue for model 5

- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



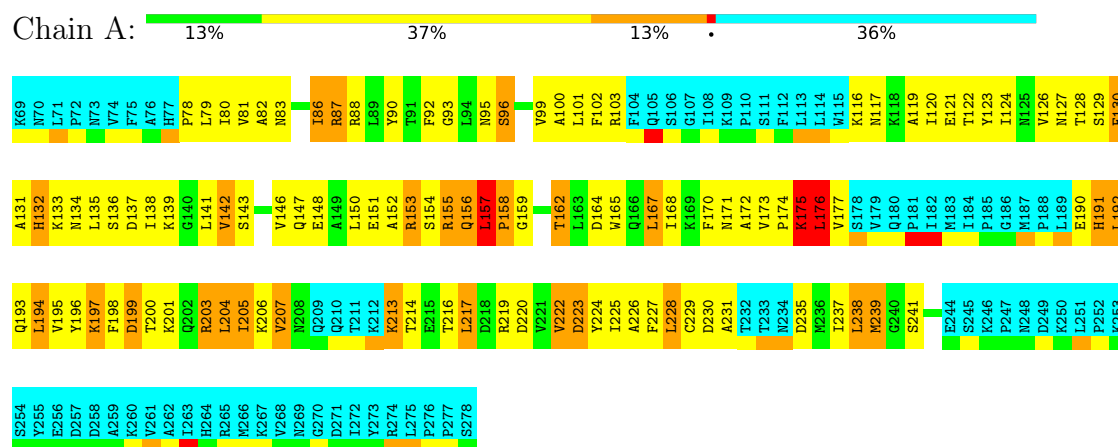
4.2.6 Score per residue for model 6

- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



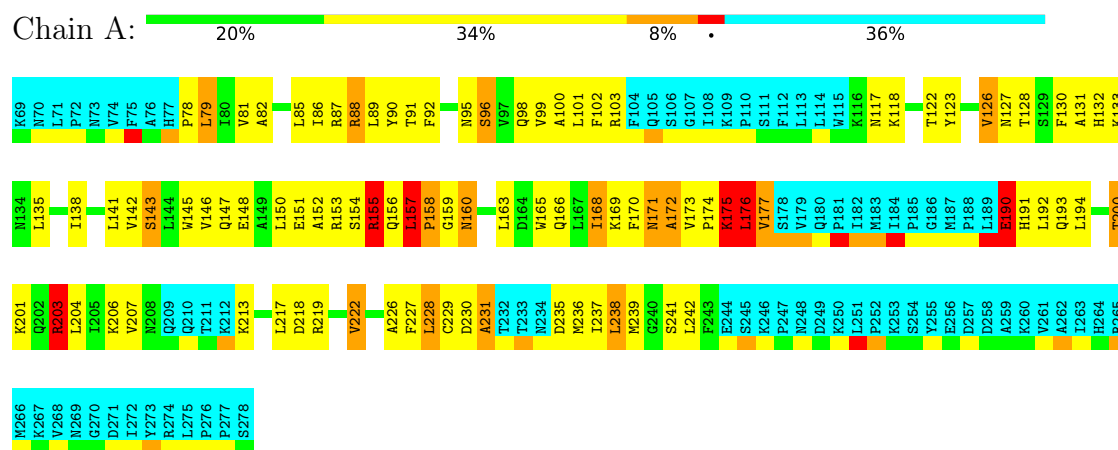
4.2.7 Score per residue for model 7

- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



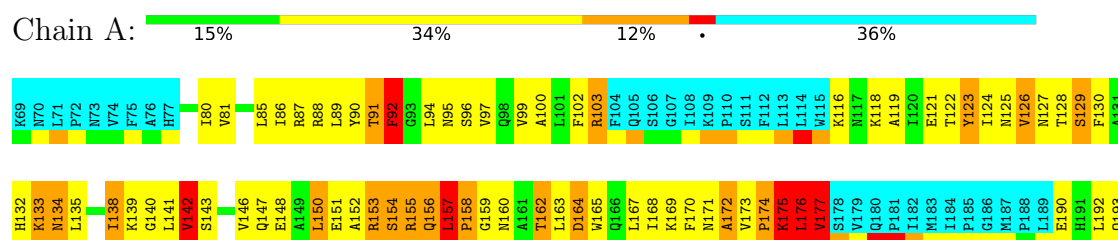
4.2.8 Score per residue for model 8

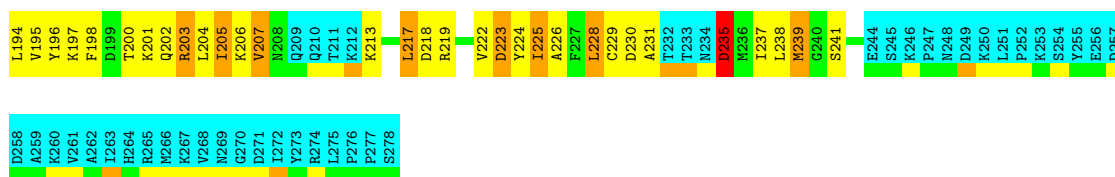
- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



4.2.9 Score per residue for model 9

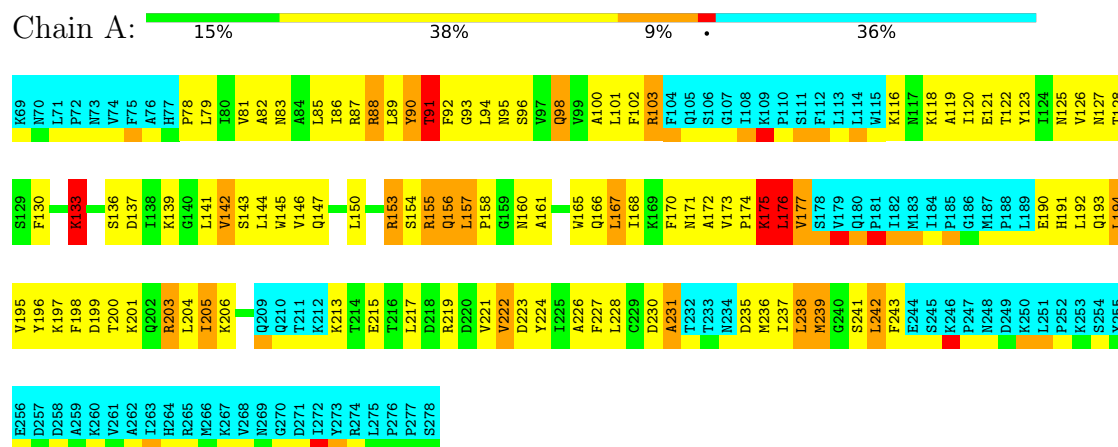
- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial





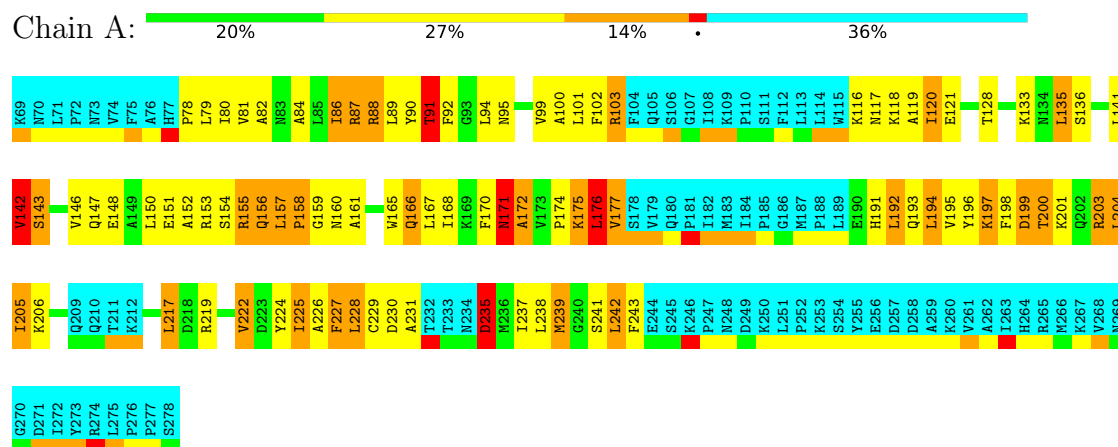
4.2.10 Score per residue for model 10

- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



4.2.11 Score per residue for model 11

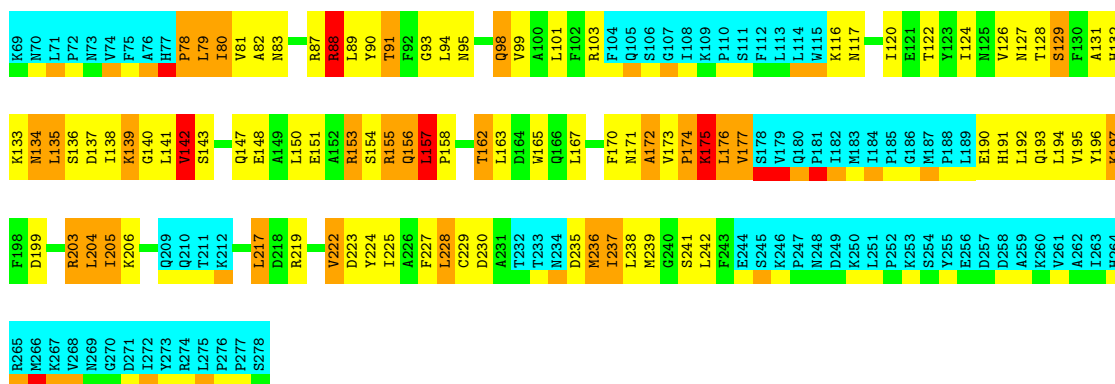
- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



4.2.12 Score per residue for model 12

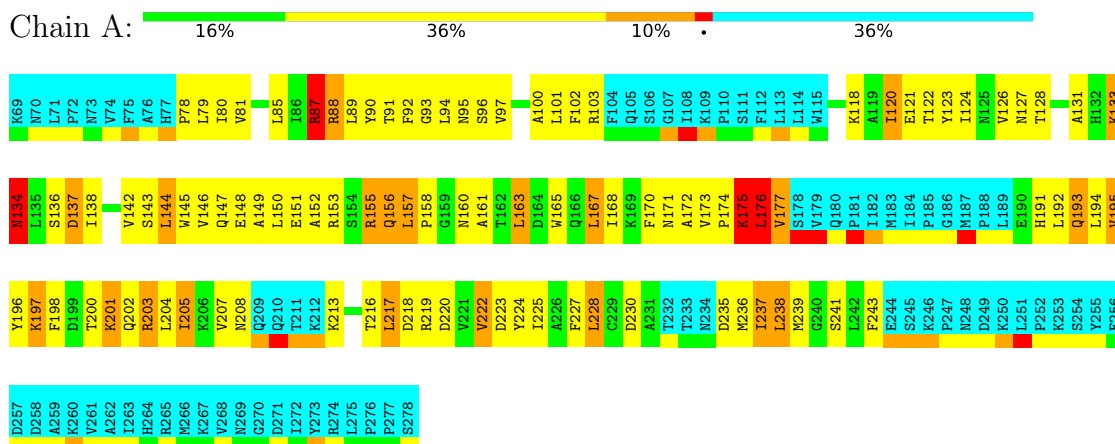
- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial





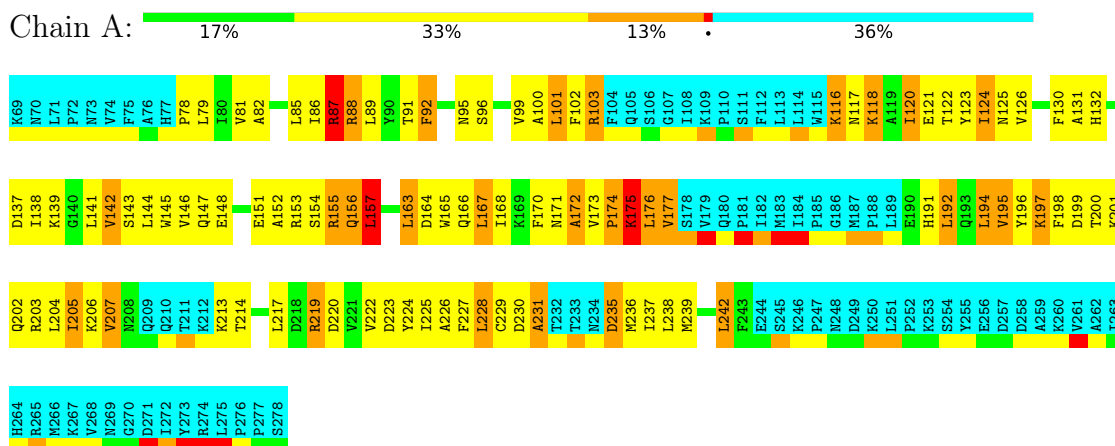
4.2.13 Score per residue for model 13

- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



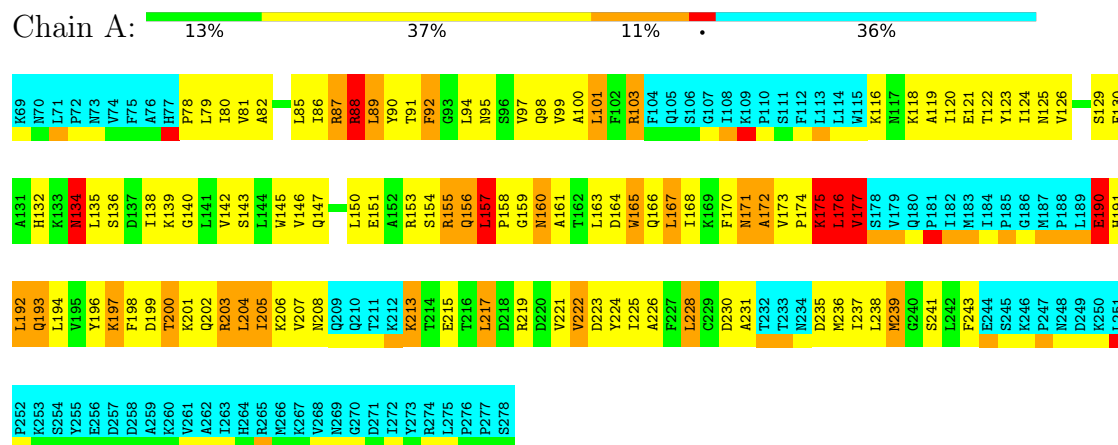
4.2.14 Score per residue for model 14

- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



4.2.15 Score per residue for model 15

- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	2.19
X-PLOR NIH	refinement	2.19

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	1586
Number of shifts mapped to atoms	1469
Number of unparsed shifts	0
Number of shifts with mapping errors	117
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.50±0.02	2±1/1110 (0.2± 0.1%)	1.95±0.08	17±2/1504 (1.1± 0.1%)
All	All	1.50	37/16650 (0.2%)	1.95	259/22560 (1.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	9.5±1.1
All	All	0	142

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	176	LEU	C-N	13.62	1.52	1.33	9	9
1	A	175	LYS	C-N	12.27	1.50	1.33	13	15
1	A	177	VAL	CA-CB	8.36	1.65	1.54	7	1
1	A	175	LYS	N-CA	8.29	1.55	1.46	3	6
1	A	176	LEU	N-CA	6.82	1.54	1.46	8	1
1	A	176	LEU	CA-C	5.58	1.59	1.52	4	2
1	A	177	VAL	C-N	5.50	1.41	1.33	5	1
1	A	175	LYS	CA-C	-5.50	1.45	1.52	4	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	177	VAL	N-CA-C	27.22	145.56	108.27	1	8
1	A	176	LEU	N-CA-C	26.39	152.42	109.40	14	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	175	LYS	N-CA-C	22.66	145.49	108.32	13	15
1	A	176	LEU	CA-C-N	-13.17	104.64	122.94	15	15
1	A	176	LEU	C-N-CA	-13.17	104.64	122.94	15	15
1	A	177	VAL	N-CA-CB	-11.44	94.82	111.52	7	13
1	A	175	LYS	CA-C-N	-11.34	102.87	122.37	10	15
1	A	175	LYS	C-N-CA	-11.34	102.87	122.37	10	15
1	A	176	LEU	N-CA-CB	-11.11	91.59	110.80	9	15
1	A	177	VAL	CA-C-N	-9.34	109.60	122.77	9	11
1	A	177	VAL	C-N-CA	-9.34	109.60	122.77	9	11
1	A	175	LYS	N-CA-CB	-8.84	95.55	110.49	10	15
1	A	174	PRO	CA-C-N	-8.02	108.00	121.64	5	11
1	A	174	PRO	C-N-CA	-8.02	108.00	121.64	5	11
1	A	177	VAL	CB-CA-C	-7.28	99.35	111.29	9	8
1	A	176	LEU	CB-CA-C	-7.11	98.77	110.14	12	10
1	A	176	LEU	CA-C-O	6.50	128.13	120.66	2	2
1	A	175	LYS	CB-CA-C	-6.50	99.53	109.99	7	6
1	A	160	ASN	N-CA-CB	-5.67	104.98	111.79	10	2
1	A	205	ILE	N-CA-CB	-5.53	105.16	112.34	10	11
1	A	207	VAL	N-CA-CB	-5.50	105.05	112.10	9	5
1	A	195	VAL	N-CA-CB	-5.50	104.75	111.67	5	6
1	A	175	LYS	CA-C-O	5.46	126.80	120.14	3	4
1	A	126	VAL	N-CA-CB	-5.34	105.01	110.62	8	4
1	A	174	PRO	CA-C-O	-5.33	114.79	122.31	5	1
1	A	222	VAL	N-CA-CB	-5.32	104.97	111.67	2	12
1	A	138	ILE	N-CA-CB	-5.19	104.96	110.62	5	1
1	A	120	ILE	N-CA-CB	-5.11	105.05	110.62	14	1
1	A	81	VAL	N-CA-CB	-5.07	105.09	110.62	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	87	ARG	Sidechain	15
1	A	88	ARG	Sidechain	15
1	A	103	ARG	Sidechain	15
1	A	153	ARG	Sidechain	15
1	A	155	ARG	Sidechain	15
1	A	203	ARG	Sidechain	15
1	A	219	ARG	Sidechain	15
1	A	175	LYS	Mainchain,Peptide	14

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	176	LEU	Peptide,Mainchain	7
1	A	177	VAL	Mainchain	7

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1090	1135	1135	117±19
All	All	16350	17025	17025	1757

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 53.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:LEU:HD22	1:A:196:TYR:CD2	1.01	1.90	1	2
1:A:126:VAL:HG21	1:A:238:LEU:HD13	1.01	1.22	5	1
1:A:144:LEU:HD13	1:A:145:TRP:N	1.00	1.71	13	1
1:A:122:THR:HG21	1:A:236:MET:HE1	0.99	1.33	5	1
1:A:242:LEU:O	1:A:242:LEU:HD13	0.99	1.58	11	1
1:A:228:LEU:HD11	1:A:237:ILE:HG21	0.96	1.36	9	1
1:A:138:ILE:O	1:A:142:VAL:HG22	0.95	1.61	13	2
1:A:226:ALA:HB3	1:A:239:MET:O	0.95	1.60	8	3
1:A:199:ASP:CG	1:A:222:VAL:HG12	0.95	1.86	6	2
1:A:126:VAL:CG2	1:A:238:LEU:HD13	0.94	1.93	5	1
1:A:89:LEU:O	1:A:91:THR:HG23	0.94	1.63	6	1
1:A:131:ALA:HB1	1:A:163:LEU:O	0.93	1.63	1	6
1:A:146:VAL:HG11	1:A:238:LEU:HD23	0.93	1.39	6	1
1:A:228:LEU:HB2	1:A:237:ILE:HD11	0.89	1.42	13	2
1:A:87:ARG:O	1:A:91:THR:HG22	0.89	1.68	14	2
1:A:193:GLN:CD	1:A:228:LEU:HD11	0.87	1.94	8	1
1:A:140:GLY:O	1:A:142:VAL:HG23	0.87	1.68	15	2
1:A:162:THR:O	1:A:163:LEU:HD22	0.87	1.70	6	1
1:A:176:LEU:HD21	1:A:195:VAL:O	0.87	1.69	10	1
1:A:78:PRO:O	1:A:81:VAL:HG12	0.86	1.69	13	5
1:A:94:LEU:HD12	1:A:95:ASN:N	0.86	1.84	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:242:LEU:HD22	1:A:243:PHE:N	0.86	1.86	11	1
1:A:141:LEU:O	1:A:237:ILE:HG23	0.86	1.69	10	3
1:A:124:ILE:HA	1:A:167:LEU:HD13	0.86	1.46	7	1
1:A:242:LEU:C	1:A:242:LEU:HD22	0.85	1.96	2	1
1:A:228:LEU:HD22	1:A:237:ILE:HD12	0.85	1.46	3	1
1:A:176:LEU:HD23	1:A:197:LYS:HB2	0.85	1.47	15	1
1:A:101:LEU:O	1:A:101:LEU:HD13	0.85	1.72	14	2
1:A:195:VAL:HG13	1:A:224:TYR:CZ	0.84	2.07	14	2
1:A:225:ILE:HD13	1:A:241:SER:HB3	0.84	1.49	4	1
1:A:228:LEU:HD12	1:A:239:MET:SD	0.84	2.13	4	2
1:A:167:LEU:O	1:A:167:LEU:HD23	0.84	1.71	15	1
1:A:198:PHE:CZ	1:A:200:THR:HG21	0.83	2.07	3	3
1:A:80:ILE:HD13	1:A:80:ILE:O	0.83	1.72	2	1
1:A:79:LEU:C	1:A:79:LEU:HD22	0.83	1.98	12	2
1:A:120:ILE:HD13	1:A:120:ILE:O	0.83	1.72	4	1
1:A:164:ASP:CB	1:A:205:ILE:HD11	0.83	2.03	14	3
1:A:228:LEU:HD11	1:A:237:ILE:CG2	0.83	2.04	9	1
1:A:154:SER:O	1:A:157:LEU:HD12	0.83	1.74	2	4
1:A:78:PRO:O	1:A:81:VAL:HG22	0.83	1.72	8	4
1:A:126:VAL:HG22	1:A:238:LEU:CD2	0.83	2.04	9	1
1:A:126:VAL:HG21	1:A:238:LEU:CD1	0.82	2.04	5	1
1:A:122:THR:HG21	1:A:236:MET:CE	0.82	2.03	5	1
1:A:164:ASP:HB2	1:A:205:ILE:HD11	0.82	1.48	14	2
1:A:138:ILE:HD12	1:A:150:LEU:HD23	0.81	1.48	12	1
1:A:228:LEU:HD23	1:A:237:ILE:HD12	0.81	1.51	1	1
1:A:163:LEU:C	1:A:163:LEU:HD22	0.81	2.00	2	1
1:A:204:LEU:C	1:A:205:ILE:HD12	0.81	2.00	15	1
1:A:128:THR:HG23	1:A:165:TRP:CD1	0.81	2.11	10	2
1:A:86:ILE:HD13	1:A:86:ILE:O	0.81	1.75	11	2
1:A:199:ASP:OD2	1:A:222:VAL:HG12	0.81	1.75	12	1
1:A:224:TYR:C	1:A:225:ILE:HD12	0.80	2.00	6	1
1:A:228:LEU:CB	1:A:237:ILE:HD11	0.80	2.05	13	1
1:A:124:ILE:CD1	1:A:167:LEU:HD21	0.80	2.06	14	1
1:A:195:VAL:HG13	1:A:224:TYR:CE2	0.80	2.12	14	1
1:A:167:LEU:HD21	1:A:200:THR:CG2	0.80	2.06	10	1
1:A:157:LEU:C	1:A:157:LEU:HD22	0.80	2.02	2	2
1:A:176:LEU:HD11	1:A:196:TYR:CD2	0.80	2.12	12	1
1:A:176:LEU:HD12	1:A:176:LEU:O	0.79	1.78	9	2
1:A:90:TYR:O	1:A:91:THR:HG23	0.79	1.78	11	1
1:A:168:ILE:HD12	1:A:202:GLN:HA	0.79	1.50	3	1
1:A:144:LEU:C	1:A:144:LEU:HD22	0.79	2.03	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:199:ASP:OD1	1:A:222:VAL:HG22	0.78	1.76	14	2
1:A:242:LEU:HD22	1:A:242:LEU:C	0.78	2.02	11	1
1:A:141:LEU:HD23	1:A:238:LEU:HB2	0.78	1.54	10	3
1:A:141:LEU:O	1:A:142:VAL:HG13	0.78	1.76	9	2
1:A:124:ILE:HD12	1:A:167:LEU:HD21	0.78	1.55	14	1
1:A:130:PHE:CE1	1:A:150:LEU:HD23	0.78	2.13	1	1
1:A:146:VAL:HG21	1:A:238:LEU:HD23	0.78	1.54	2	2
1:A:131:ALA:HB2	1:A:165:TRP:HB2	0.78	1.56	7	1
1:A:207:VAL:HG23	1:A:213:LYS:O	0.78	1.79	13	1
1:A:193:GLN:C	1:A:194:LEU:HD12	0.77	2.04	12	3
1:A:175:LYS:HA	1:A:176:LEU:HD12	0.77	1.55	4	2
1:A:101:LEU:HD23	1:A:102:PHE:N	0.77	1.93	8	2
1:A:122:THR:HG21	1:A:236:MET:SD	0.77	2.20	10	3
1:A:191:HIS:C	1:A:192:LEU:HD12	0.77	2.04	10	1
1:A:228:LEU:O	1:A:237:ILE:HD12	0.77	1.78	10	2
1:A:158:PRO:HG2	1:A:161:ALA:HB3	0.76	1.56	2	1
1:A:88:ARG:HA	1:A:91:THR:HG23	0.76	1.58	12	1
1:A:91:THR:HG22	1:A:94:LEU:HD21	0.76	1.57	10	1
1:A:167:LEU:HD13	1:A:168:ILE:N	0.76	1.96	10	1
1:A:228:LEU:HD23	1:A:237:ILE:CD1	0.75	2.12	1	1
1:A:126:VAL:HG13	1:A:238:LEU:HD22	0.75	1.56	9	1
1:A:176:LEU:HD13	1:A:195:VAL:O	0.75	1.81	9	1
1:A:144:LEU:HD22	1:A:144:LEU:O	0.74	1.81	13	1
1:A:148:GLU:O	1:A:152:ALA:HB2	0.74	1.81	11	6
1:A:157:LEU:HD23	1:A:158:PRO:HD2	0.74	1.59	10	3
1:A:167:LEU:HD21	1:A:200:THR:HG21	0.74	1.57	10	1
1:A:176:LEU:HD23	1:A:177:VAL:HA	0.74	1.58	8	2
1:A:167:LEU:HD11	1:A:200:THR:CG2	0.74	2.11	10	1
1:A:167:LEU:HD11	1:A:200:THR:OG1	0.73	1.82	10	1
1:A:161:ALA:HB1	1:A:207:VAL:O	0.73	1.83	3	2
1:A:154:SER:O	1:A:157:LEU:HD23	0.73	1.83	6	2
1:A:122:THR:O	1:A:126:VAL:HG23	0.73	1.84	2	5
1:A:122:THR:HG21	1:A:141:LEU:HD12	0.72	1.60	2	1
1:A:154:SER:O	1:A:157:LEU:HD13	0.72	1.83	14	1
1:A:165:TRP:O	1:A:167:LEU:HD12	0.72	1.85	1	1
1:A:145:TRP:HB2	1:A:239:MET:HE2	0.72	1.61	5	1
1:A:176:LEU:O	1:A:177:VAL:HG13	0.72	1.85	9	2
1:A:138:ILE:HD11	1:A:147:GLN:HG3	0.72	1.62	7	1
1:A:192:LEU:O	1:A:228:LEU:HD12	0.72	1.83	14	1
1:A:123:TYR:CE1	1:A:225:ILE:HD13	0.72	2.19	15	1
1:A:176:LEU:HD22	1:A:195:VAL:O	0.71	1.85	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:LEU:HD13	1:A:239:MET:SD	0.71	2.25	6	2
1:A:150:LEU:C	1:A:150:LEU:HD23	0.71	2.10	11	2
1:A:176:LEU:HD23	1:A:197:LYS:CB	0.71	2.15	15	1
1:A:126:VAL:HG11	1:A:238:LEU:HG	0.71	1.62	13	1
1:A:176:LEU:O	1:A:176:LEU:HD23	0.71	1.86	5	1
1:A:165:TRP:CD2	1:A:204:LEU:HD12	0.70	2.21	2	1
1:A:79:LEU:HD22	1:A:80:ILE:N	0.70	2.00	12	2
1:A:167:LEU:HD12	1:A:198:PHE:CZ	0.70	2.21	15	1
1:A:85:LEU:HD23	1:A:86:ILE:N	0.70	2.01	8	5
1:A:146:VAL:HG12	1:A:150:LEU:HD12	0.70	1.61	8	1
1:A:90:TYR:O	1:A:92:PHE:N	0.70	2.23	10	3
1:A:89:LEU:O	1:A:89:LEU:HD23	0.70	1.87	8	2
1:A:120:ILE:HG23	1:A:198:PHE:CD1	0.70	2.21	14	1
1:A:122:THR:CG2	1:A:236:MET:HE1	0.70	2.13	5	1
1:A:101:LEU:HD23	1:A:101:LEU:C	0.70	2.12	8	3
1:A:126:VAL:HG11	1:A:238:LEU:CD1	0.70	2.16	15	1
1:A:162:THR:C	1:A:163:LEU:HD12	0.70	2.10	12	1
1:A:120:ILE:HG22	1:A:198:PHE:CE2	0.70	2.21	13	1
1:A:144:LEU:HD11	1:A:145:TRP:NE1	0.70	2.01	14	1
1:A:195:VAL:HG12	1:A:224:TYR:CE1	0.70	2.21	4	1
1:A:230:ASP:O	1:A:231:ALA:HB2	0.70	1.87	8	3
1:A:242:LEU:HD13	1:A:242:LEU:C	0.70	2.11	11	1
1:A:237:ILE:C	1:A:237:ILE:HD12	0.70	2.12	12	1
1:A:225:ILE:HG23	1:A:240:GLY:HA3	0.69	1.63	5	1
1:A:82:ALA:O	1:A:86:ILE:HG22	0.69	1.87	15	2
1:A:225:ILE:HG22	1:A:241:SER:HB3	0.69	1.64	7	1
1:A:130:PHE:CZ	1:A:150:LEU:HD23	0.69	2.23	7	2
1:A:191:HIS:HB3	1:A:228:LEU:HD12	0.69	1.65	2	1
1:A:126:VAL:HG22	1:A:141:LEU:HD11	0.68	1.66	6	1
1:A:142:VAL:HG12	1:A:238:LEU:CB	0.68	2.18	2	1
1:A:157:LEU:HD22	1:A:158:PRO:N	0.68	2.03	2	2
1:A:195:VAL:O	1:A:195:VAL:HG13	0.68	1.89	13	3
1:A:176:LEU:O	1:A:177:VAL:CG1	0.67	2.42	9	2
1:A:176:LEU:C	1:A:177:VAL:HG13	0.67	2.13	9	6
1:A:89:LEU:HD23	1:A:89:LEU:C	0.67	2.14	8	1
1:A:135:LEU:O	1:A:138:ILE:HG22	0.67	1.89	7	3
1:A:204:LEU:C	1:A:204:LEU:HD23	0.67	2.14	2	1
1:A:167:LEU:HD11	1:A:200:THR:HG21	0.66	1.66	10	1
1:A:217:LEU:C	1:A:217:LEU:HD23	0.66	2.15	1	1
1:A:93:GLY:O	1:A:97:VAL:HG23	0.66	1.91	4	3
1:A:171:ASN:O	1:A:172:ALA:HB2	0.66	1.89	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:199:ASP:CG	1:A:222:VAL:HG22	0.66	2.15	3	2
1:A:126:VAL:HG11	1:A:238:LEU:HD11	0.66	1.68	15	1
1:A:124:ILE:CG1	1:A:167:LEU:HD21	0.66	2.21	14	1
1:A:86:ILE:HD13	1:A:86:ILE:C	0.65	2.16	11	2
1:A:205:ILE:O	1:A:205:ILE:HG23	0.65	1.91	1	4
1:A:101:LEU:HD12	1:A:101:LEU:C	0.65	2.17	4	1
1:A:124:ILE:HG22	1:A:167:LEU:HD11	0.65	1.69	4	2
1:A:193:GLN:NE2	1:A:228:LEU:HD11	0.65	2.06	8	1
1:A:230:ASP:O	1:A:231:ALA:HB3	0.65	1.91	1	5
1:A:80:ILE:N	1:A:80:ILE:HD12	0.65	2.05	6	1
1:A:80:ILE:HD13	1:A:80:ILE:C	0.65	2.16	2	1
1:A:131:ALA:HB2	1:A:165:TRP:CD1	0.65	2.27	12	4
1:A:228:LEU:HD13	1:A:239:MET:CG	0.65	2.21	6	1
1:A:228:LEU:HD23	1:A:237:ILE:HB	0.65	1.68	15	1
1:A:222:VAL:HG23	1:A:222:VAL:O	0.65	1.91	15	2
1:A:144:LEU:HD13	1:A:145:TRP:H	0.65	1.52	13	1
1:A:90:TYR:CD1	1:A:92:PHE:CD1	0.65	2.85	4	1
1:A:222:VAL:O	1:A:222:VAL:HG23	0.65	1.90	12	5
1:A:163:LEU:HD22	1:A:163:LEU:O	0.64	1.91	2	1
1:A:94:LEU:HD12	1:A:94:LEU:C	0.64	2.17	10	2
1:A:195:VAL:CG1	1:A:224:TYR:CZ	0.64	2.80	6	1
1:A:78:PRO:O	1:A:81:VAL:HG13	0.64	1.92	10	1
1:A:135:LEU:C	1:A:135:LEU:HD23	0.64	2.16	3	2
1:A:177:VAL:HA	1:A:195:VAL:HG12	0.64	1.68	1	1
1:A:197:LYS:CG	1:A:224:TYR:CD1	0.64	2.81	9	3
1:A:120:ILE:HD13	1:A:120:ILE:C	0.64	2.16	4	1
1:A:197:LYS:CG	1:A:224:TYR:CD2	0.64	2.80	13	3
1:A:198:PHE:CE1	1:A:225:ILE:CD1	0.64	2.81	5	1
1:A:138:ILE:HG23	1:A:142:VAL:HG21	0.64	1.69	8	1
1:A:177:VAL:O	1:A:177:VAL:HG13	0.64	1.93	15	1
1:A:85:LEU:C	1:A:85:LEU:HD23	0.63	2.18	5	4
1:A:197:LYS:HD3	1:A:222:VAL:HG23	0.63	1.70	2	1
1:A:146:VAL:HG21	1:A:239:MET:HA	0.63	1.70	14	4
1:A:195:VAL:HG11	1:A:224:TYR:CZ	0.63	2.28	6	1
1:A:124:ILE:HG22	1:A:167:LEU:CD1	0.63	2.23	6	2
1:A:195:VAL:CG1	1:A:224:TYR:CE2	0.63	2.81	14	1
1:A:207:VAL:O	1:A:207:VAL:HG13	0.63	1.94	7	1
1:A:123:TYR:CE1	1:A:225:ILE:HD12	0.63	2.29	1	1
1:A:146:VAL:HG11	1:A:238:LEU:HD22	0.63	1.71	2	1
1:A:144:LEU:HD13	1:A:144:LEU:C	0.63	2.18	13	1
1:A:222:VAL:O	1:A:222:VAL:HG13	0.63	1.92	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:ARG:O	1:A:157:LEU:HD13	0.62	1.94	2	1
1:A:79:LEU:C	1:A:79:LEU:CD2	0.62	2.72	12	2
1:A:228:LEU:HD23	1:A:237:ILE:CG1	0.62	2.23	15	1
1:A:135:LEU:HD23	1:A:135:LEU:O	0.62	1.93	4	3
1:A:198:PHE:O	1:A:198:PHE:CG	0.62	2.52	5	1
1:A:228:LEU:HD23	1:A:237:ILE:CB	0.62	2.24	15	1
1:A:224:TYR:CD1	1:A:224:TYR:N	0.62	2.66	2	4
1:A:158:PRO:HG3	1:A:161:ALA:HB3	0.62	1.71	10	2
1:A:126:VAL:HG11	1:A:238:LEU:HD22	0.62	1.70	5	1
1:A:168:ILE:HD12	1:A:201:LYS:HB3	0.62	1.71	9	2
1:A:123:TYR:CE1	1:A:225:ILE:CD1	0.62	2.82	1	1
1:A:198:PHE:CZ	1:A:200:THR:CG2	0.62	2.82	6	2
1:A:124:ILE:HA	1:A:167:LEU:HD22	0.62	1.68	14	3
1:A:241:SER:O	1:A:242:LEU:HD22	0.62	1.94	10	1
1:A:101:LEU:HD23	1:A:101:LEU:O	0.62	1.94	12	1
1:A:120:ILE:CG2	1:A:198:PHE:CE2	0.62	2.83	13	1
1:A:158:PRO:CG	1:A:161:ALA:HB3	0.61	2.25	10	3
1:A:195:VAL:HG13	1:A:224:TYR:OH	0.61	1.94	14	1
1:A:85:LEU:HD23	1:A:85:LEU:C	0.61	2.19	8	2
1:A:176:LEU:HD23	1:A:176:LEU:O	0.61	1.95	8	2
1:A:141:LEU:O	1:A:142:VAL:HG22	0.61	1.96	3	1
1:A:175:LYS:O	1:A:176:LEU:HD23	0.61	1.96	13	1
1:A:123:TYR:CD2	1:A:198:PHE:CE2	0.61	2.88	14	1
1:A:224:TYR:CD2	1:A:224:TYR:N	0.61	2.67	13	2
1:A:165:TRP:CE2	1:A:204:LEU:HD12	0.61	2.31	2	1
1:A:177:VAL:HG12	1:A:195:VAL:HB	0.61	1.71	14	1
1:A:90:TYR:CE1	1:A:92:PHE:CD1	0.61	2.89	4	1
1:A:176:LEU:HD23	1:A:176:LEU:C	0.60	2.21	5	2
1:A:221:VAL:HG22	1:A:223:ASP:OD1	0.60	1.97	10	1
1:A:157:LEU:HD22	1:A:158:PRO:C	0.60	2.22	2	2
1:A:242:LEU:HD22	1:A:243:PHE:CB	0.60	2.26	2	1
1:A:198:PHE:CE1	1:A:225:ILE:HD11	0.60	2.32	5	1
1:A:150:LEU:HD23	1:A:151:GLU:N	0.60	2.11	11	1
1:A:225:ILE:HD13	1:A:241:SER:CB	0.60	2.26	4	1
1:A:124:ILE:O	1:A:128:THR:HG23	0.60	1.97	13	1
1:A:91:THR:HG23	1:A:91:THR:O	0.60	1.95	15	1
1:A:222:VAL:HG13	1:A:222:VAL:O	0.60	1.97	2	2
1:A:177:VAL:CA	1:A:195:VAL:HG12	0.60	2.27	1	1
1:A:191:HIS:CD2	1:A:228:LEU:HD21	0.59	2.32	15	1
1:A:85:LEU:C	1:A:85:LEU:HD13	0.59	2.22	1	1
1:A:177:VAL:C	1:A:195:VAL:HG12	0.59	2.22	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:ASN:ND2	1:A:165:TRP:CE3	0.59	2.70	1	2
1:A:196:TYR:CE2	1:A:225:ILE:HG22	0.59	2.32	5	1
1:A:131:ALA:HB2	1:A:165:TRP:HD1	0.59	1.58	13	2
1:A:224:TYR:N	1:A:224:TYR:CD2	0.59	2.68	12	3
1:A:138:ILE:C	1:A:142:VAL:HG22	0.59	2.21	13	1
1:A:135:LEU:C	1:A:135:LEU:HD12	0.59	2.23	2	1
1:A:144:LEU:HD11	1:A:145:TRP:CE3	0.59	2.33	2	1
1:A:163:LEU:CD1	1:A:163:LEU:N	0.58	2.66	2	1
1:A:145:TRP:CB	1:A:239:MET:HE2	0.58	2.28	5	1
1:A:172:ALA:HB1	1:A:199:ASP:CG	0.58	2.23	15	1
1:A:191:HIS:O	1:A:192:LEU:HD12	0.58	1.97	10	1
1:A:123:TYR:CZ	1:A:198:PHE:CD2	0.58	2.91	1	1
1:A:192:LEU:O	1:A:228:LEU:HD13	0.58	1.96	2	1
1:A:173:VAL:HG11	1:A:197:LYS:O	0.58	1.98	7	1
1:A:194:LEU:HD12	1:A:196:TYR:CZ	0.58	2.33	14	1
1:A:142:VAL:HG13	1:A:142:VAL:O	0.58	1.99	11	1
1:A:198:PHE:CD1	1:A:225:ILE:CD1	0.58	2.87	5	1
1:A:172:ALA:HB1	1:A:199:ASP:HB3	0.58	1.76	11	1
1:A:92:PHE:CG	1:A:92:PHE:O	0.58	2.57	14	3
1:A:135:LEU:HD12	1:A:136:SER:N	0.58	2.14	2	1
1:A:88:ARG:CD	1:A:92:PHE:CE2	0.58	2.86	11	1
1:A:94:LEU:HD22	1:A:94:LEU:N	0.58	2.14	13	1
1:A:227:PHE:CD1	1:A:227:PHE:C	0.57	2.81	6	1
1:A:144:LEU:HD11	1:A:145:TRP:CD1	0.57	2.34	14	1
1:A:192:LEU:HD12	1:A:229:CYS:O	0.57	2.00	9	3
1:A:163:LEU:C	1:A:163:LEU:CD2	0.57	2.75	2	1
1:A:99:VAL:O	1:A:102:PHE:CD1	0.57	2.58	5	1
1:A:176:LEU:HD11	1:A:224:TYR:HB3	0.57	1.74	15	1
1:A:90:TYR:C	1:A:91:THR:HG22	0.57	2.24	4	1
1:A:173:VAL:HG13	1:A:174:PRO:HD2	0.57	1.76	6	4
1:A:119:ALA:O	1:A:123:TYR:CD2	0.57	2.58	15	1
1:A:168:ILE:N	1:A:202:GLN:HB2	0.57	2.14	15	1
1:A:172:ALA:C	1:A:173:VAL:HG23	0.57	2.23	15	3
1:A:120:ILE:HD11	1:A:169:LYS:HE3	0.57	1.75	3	1
1:A:130:PHE:CE1	1:A:150:LEU:HD12	0.57	2.35	4	1
1:A:192:LEU:O	1:A:228:LEU:HD23	0.57	1.99	12	2
1:A:224:TYR:C	1:A:224:TYR:CD2	0.57	2.81	6	1
1:A:157:LEU:HD13	1:A:157:LEU:O	0.57	2.00	2	2
1:A:157:LEU:CD1	1:A:157:LEU:N	0.57	2.67	5	2
1:A:176:LEU:CD1	1:A:195:VAL:O	0.57	2.52	9	2
1:A:92:PHE:CD1	1:A:92:PHE:C	0.57	2.82	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:LEU:HD13	1:A:79:LEU:O	0.57	1.98	6	1
1:A:126:VAL:HG22	1:A:238:LEU:HD21	0.57	1.74	9	1
1:A:203:ARG:CB	1:A:217:LEU:O	0.57	2.53	15	2
1:A:94:LEU:CD1	1:A:95:ASN:N	0.57	2.68	10	3
1:A:162:THR:HB	1:A:207:VAL:HG12	0.57	1.75	7	1
1:A:196:TYR:CE1	1:A:197:LYS:O	0.57	2.58	7	1
1:A:120:ILE:O	1:A:124:ILE:HG22	0.57	1.99	12	1
1:A:228:LEU:C	1:A:228:LEU:HD23	0.57	2.24	3	1
1:A:168:ILE:CB	1:A:202:GLN:HB2	0.57	2.29	15	1
1:A:92:PHE:CZ	1:A:95:ASN:ND2	0.56	2.73	2	1
1:A:196:TYR:CE2	1:A:225:ILE:CG2	0.56	2.87	5	1
1:A:214:THR:O	1:A:214:THR:HG23	0.56	1.99	5	1
1:A:130:PHE:CE1	1:A:150:LEU:CD2	0.56	2.89	8	2
1:A:195:VAL:CG1	1:A:195:VAL:O	0.56	2.53	1	1
1:A:168:ILE:HD12	1:A:202:GLN:CA	0.56	2.29	3	1
1:A:79:LEU:N	1:A:79:LEU:HD13	0.56	2.15	4	2
1:A:176:LEU:CB	1:A:195:VAL:O	0.56	2.54	9	2
1:A:146:VAL:HG23	1:A:239:MET:C	0.56	2.25	13	4
1:A:195:VAL:CG1	1:A:224:TYR:CE1	0.56	2.89	4	2
1:A:228:LEU:HD13	1:A:239:MET:HG2	0.56	1.76	6	1
1:A:155:ARG:CD	1:A:156:GLN:N	0.56	2.68	8	1
1:A:224:TYR:C	1:A:224:TYR:CD1	0.56	2.82	14	1
1:A:132:HIS:O	1:A:132:HIS:CD2	0.56	2.59	7	1
1:A:173:VAL:CG2	1:A:197:LYS:CD	0.56	2.84	7	1
1:A:163:LEU:HD21	1:A:206:LYS:CD	0.56	2.30	9	1
1:A:228:LEU:CB	1:A:237:ILE:CD1	0.56	2.82	13	1
1:A:95:ASN:O	1:A:99:VAL:HG12	0.56	1.99	14	1
1:A:176:LEU:HD22	1:A:196:TYR:CE2	0.56	2.34	1	1
1:A:197:LYS:HG3	1:A:224:TYR:CD1	0.56	2.35	1	4
1:A:138:ILE:HG22	1:A:142:VAL:HG21	0.56	1.77	13	1
1:A:95:ASN:ND2	1:A:99:VAL:HG21	0.56	2.16	4	1
1:A:91:THR:CG2	1:A:94:LEU:HD21	0.56	2.28	10	1
1:A:197:LYS:HG2	1:A:224:TYR:CD2	0.56	2.36	13	3
1:A:124:ILE:CG1	1:A:167:LEU:HD22	0.56	2.31	15	1
1:A:197:LYS:HG2	1:A:224:TYR:CD1	0.56	2.35	9	2
1:A:228:LEU:CD2	1:A:237:ILE:HD12	0.56	2.25	3	1
1:A:177:VAL:O	1:A:195:VAL:CG1	0.56	2.54	6	1
1:A:126:VAL:CG2	1:A:238:LEU:CD2	0.56	2.82	9	2
1:A:84:ALA:HB1	1:A:88:ARG:NH1	0.56	2.16	11	1
1:A:130:PHE:CE2	1:A:150:LEU:CD2	0.55	2.88	3	1
1:A:79:LEU:N	1:A:79:LEU:CD1	0.55	2.70	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:ASN:ND2	1:A:128:THR:N	0.55	2.54	4	1
1:A:138:ILE:CD1	1:A:150:LEU:HD23	0.55	2.31	15	2
1:A:196:TYR:CD1	1:A:196:TYR:C	0.55	2.84	7	1
1:A:99:VAL:O	1:A:102:PHE:CZ	0.55	2.60	2	1
1:A:163:LEU:HD13	1:A:163:LEU:H	0.55	1.60	2	1
1:A:173:VAL:HG23	1:A:174:PRO:HD2	0.55	1.77	3	3
1:A:197:LYS:HG3	1:A:224:TYR:CD2	0.55	2.37	13	4
1:A:237:ILE:HD12	1:A:238:LEU:N	0.55	2.17	12	1
1:A:90:TYR:CD2	1:A:91:THR:N	0.55	2.75	4	1
1:A:207:VAL:HG12	1:A:213:LYS:O	0.55	2.01	5	2
1:A:176:LEU:HD21	1:A:196:TYR:CD2	0.55	2.37	13	1
1:A:131:ALA:HB1	1:A:164:ASP:HA	0.55	1.77	6	1
1:A:101:LEU:C	1:A:101:LEU:HD23	0.55	2.26	7	2
1:A:197:LYS:HG3	1:A:224:TYR:CE1	0.55	2.37	2	1
1:A:176:LEU:CD2	1:A:195:VAL:O	0.55	2.54	9	4
1:A:90:TYR:O	1:A:92:PHE:CD2	0.55	2.59	7	1
1:A:162:THR:CB	1:A:207:VAL:HG12	0.55	2.32	7	1
1:A:197:LYS:NZ	1:A:224:TYR:CZ	0.55	2.74	7	1
1:A:197:LYS:HG3	1:A:224:TYR:CG	0.55	2.37	12	2
1:A:228:LEU:O	1:A:237:ILE:N	0.55	2.40	6	4
1:A:225:ILE:CG2	1:A:227:PHE:CZ	0.55	2.90	3	1
1:A:176:LEU:O	1:A:176:LEU:CD1	0.55	2.52	9	2
1:A:124:ILE:HD12	1:A:167:LEU:HD22	0.55	1.79	15	1
1:A:168:ILE:N	1:A:202:GLN:CB	0.55	2.69	15	1
1:A:196:TYR:OH	1:A:225:ILE:HG21	0.55	2.02	4	1
1:A:190:GLU:O	1:A:191:HIS:CD2	0.55	2.60	6	2
1:A:203:ARG:CZ	1:A:216:THR:CG2	0.55	2.85	7	1
1:A:167:LEU:CD2	1:A:200:THR:HG21	0.55	2.31	10	1
1:A:202:GLN:NE2	1:A:204:LEU:HD23	0.55	2.17	15	1
1:A:242:LEU:C	1:A:242:LEU:CD2	0.55	2.71	2	2
1:A:176:LEU:HD12	1:A:195:VAL:O	0.55	2.02	5	1
1:A:228:LEU:CB	1:A:237:ILE:CG1	0.55	2.84	12	1
1:A:98:GLN:HG2	1:A:101:LEU:HD23	0.55	1.79	4	1
1:A:168:ILE:N	1:A:201:LYS:O	0.54	2.40	13	11
1:A:196:TYR:N	1:A:196:TYR:CD1	0.54	2.74	1	1
1:A:145:TRP:CD1	1:A:239:MET:HE3	0.54	2.37	10	2
1:A:174:PRO:CA	1:A:197:LYS:O	0.54	2.55	9	2
1:A:167:LEU:HD11	1:A:200:THR:CB	0.54	2.33	10	1
1:A:126:VAL:CG1	1:A:238:LEU:HD22	0.54	2.31	9	1
1:A:228:LEU:CD1	1:A:237:ILE:CG2	0.54	2.81	9	1
1:A:90:TYR:CD2	1:A:91:THR:OG1	0.54	2.60	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:LEU:O	1:A:97:VAL:HG12	0.54	2.01	15	1
1:A:174:PRO:CB	1:A:197:LYS:O	0.54	2.55	5	3
1:A:96:SER:O	1:A:100:ALA:HB2	0.54	2.01	10	1
1:A:119:ALA:O	1:A:123:TYR:CD1	0.54	2.60	9	1
1:A:144:LEU:HD11	1:A:145:TRP:CE2	0.54	2.36	14	1
1:A:163:LEU:N	1:A:163:LEU:HD13	0.54	2.17	2	1
1:A:102:PHE:CD1	1:A:103:ARG:N	0.54	2.75	5	1
1:A:164:ASP:CB	1:A:205:ILE:CG2	0.54	2.86	1	2
1:A:222:VAL:HG12	1:A:224:TYR:HE1	0.54	1.63	1	1
1:A:142:VAL:HG12	1:A:238:LEU:HB3	0.54	1.78	2	1
1:A:176:LEU:HD21	1:A:196:TYR:HD2	0.54	1.63	13	1
1:A:146:VAL:HG13	1:A:147:GLN:N	0.54	2.18	1	2
1:A:224:TYR:O	1:A:241:SER:CB	0.54	2.56	1	5
1:A:243:PHE:N	1:A:243:PHE:CD2	0.54	2.75	3	2
1:A:85:LEU:HD21	1:A:89:LEU:HD22	0.54	1.79	9	1
1:A:176:LEU:O	1:A:176:LEU:CG	0.54	2.55	15	1
1:A:126:VAL:HG23	1:A:127:ASN:N	0.54	2.18	1	1
1:A:101:LEU:HD12	1:A:102:PHE:N	0.54	2.17	4	1
1:A:207:VAL:O	1:A:207:VAL:HG23	0.54	2.02	5	2
1:A:194:LEU:HD13	1:A:195:VAL:N	0.54	2.18	6	1
1:A:195:VAL:O	1:A:195:VAL:CG1	0.54	2.56	13	2
1:A:204:LEU:O	1:A:205:ILE:HD12	0.54	2.02	15	1
1:A:207:VAL:HG13	1:A:213:LYS:O	0.54	2.03	1	2
1:A:242:LEU:HD13	1:A:242:LEU:O	0.54	2.03	2	1
1:A:196:TYR:CD2	1:A:225:ILE:O	0.54	2.61	5	1
1:A:205:ILE:HG23	1:A:205:ILE:O	0.54	2.03	10	1
1:A:141:LEU:HD12	1:A:141:LEU:N	0.54	2.18	14	1
1:A:227:PHE:N	1:A:227:PHE:CD1	0.53	2.76	13	1
1:A:168:ILE:CG1	1:A:201:LYS:O	0.53	2.57	5	5
1:A:228:LEU:HD11	1:A:239:MET:SD	0.53	2.43	10	1
1:A:146:VAL:HG13	1:A:239:MET:CG	0.53	2.33	10	1
1:A:80:ILE:N	1:A:80:ILE:CD1	0.53	2.72	6	1
1:A:197:LYS:CG	1:A:224:TYR:CG	0.53	2.92	12	1
1:A:191:HIS:HB3	1:A:228:LEU:HD21	0.53	1.79	13	1
1:A:230:ASP:O	1:A:231:ALA:CB	0.53	2.56	10	5
1:A:99:VAL:HG13	1:A:100:ALA:N	0.53	2.19	9	1
1:A:175:LYS:CE	1:A:197:LYS:O	0.53	2.57	14	1
1:A:138:ILE:HG23	1:A:139:LYS:N	0.53	2.18	9	3
1:A:195:VAL:C	1:A:196:TYR:CD1	0.53	2.87	9	1
1:A:94:LEU:N	1:A:94:LEU:CD2	0.53	2.71	13	2
1:A:197:LYS:HG2	1:A:224:TYR:CE1	0.53	2.39	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:TRP:HB2	1:A:239:MET:HE3	0.53	1.80	4	1
1:A:146:VAL:HG11	1:A:238:LEU:CD2	0.53	2.27	6	1
1:A:86:ILE:C	1:A:86:ILE:CD1	0.53	2.82	11	2
1:A:130:PHE:CE1	1:A:150:LEU:HD22	0.53	2.38	8	1
1:A:138:ILE:HD12	1:A:150:LEU:CD2	0.53	2.28	12	1
1:A:193:GLN:C	1:A:194:LEU:CD1	0.53	2.81	12	1
1:A:190:GLU:O	1:A:230:ASP:CB	0.53	2.57	10	2
1:A:198:PHE:O	1:A:198:PHE:CD2	0.53	2.62	5	1
1:A:174:PRO:O	1:A:175:LYS:HB3	0.53	2.04	12	5
1:A:194:LEU:CB	1:A:196:TYR:CE1	0.52	2.92	1	1
1:A:194:LEU:CD1	1:A:196:TYR:OH	0.52	2.57	1	1
1:A:157:LEU:C	1:A:157:LEU:CD2	0.52	2.76	5	2
1:A:228:LEU:HD22	1:A:237:ILE:CD1	0.52	2.29	3	1
1:A:147:GLN:O	1:A:151:GLU:CB	0.52	2.58	9	10
1:A:148:GLU:O	1:A:152:ALA:CB	0.52	2.57	9	6
1:A:194:LEU:O	1:A:226:ALA:HA	0.52	2.05	9	9
1:A:190:GLU:CG	1:A:190:GLU:O	0.52	2.57	7	1
1:A:81:VAL:HG23	1:A:82:ALA:N	0.52	2.19	10	1
1:A:173:VAL:CG1	1:A:199:ASP:CB	0.52	2.87	14	1
1:A:143:SER:O	1:A:147:GLN:CB	0.52	2.57	9	12
1:A:176:LEU:HB2	1:A:195:VAL:O	0.52	2.03	1	1
1:A:92:PHE:CE2	1:A:95:ASN:HB3	0.52	2.39	2	1
1:A:228:LEU:O	1:A:237:ILE:CG1	0.52	2.58	14	2
1:A:198:PHE:CE1	1:A:200:THR:OG1	0.52	2.58	2	2
1:A:192:LEU:O	1:A:228:LEU:CD2	0.52	2.58	12	1
1:A:230:ASP:CB	1:A:235:ASP:OD1	0.52	2.58	13	1
1:A:124:ILE:CD1	1:A:167:LEU:HD22	0.52	2.35	15	1
1:A:192:LEU:CB	1:A:229:CYS:O	0.52	2.57	4	1
1:A:198:PHE:CE1	1:A:225:ILE:HG13	0.52	2.40	5	1
1:A:191:HIS:CD2	1:A:228:LEU:HD11	0.52	2.40	15	1
1:A:176:LEU:C	1:A:177:VAL:CG1	0.52	2.82	8	6
1:A:157:LEU:CD2	1:A:158:PRO:O	0.52	2.58	2	1
1:A:120:ILE:C	1:A:120:ILE:CD1	0.52	2.82	4	1
1:A:204:LEU:HD22	1:A:206:LYS:HE3	0.52	1.81	10	1
1:A:197:LYS:CG	1:A:224:TYR:CE1	0.52	2.93	2	2
1:A:196:TYR:OH	1:A:225:ILE:CG2	0.52	2.58	4	1
1:A:170:PHE:O	1:A:172:ALA:N	0.52	2.43	11	2
1:A:80:ILE:C	1:A:80:ILE:CD1	0.52	2.82	2	1
1:A:92:PHE:O	1:A:96:SER:CB	0.52	2.58	10	3
1:A:143:SER:CB	1:A:146:VAL:HG12	0.52	2.35	1	1
1:A:143:SER:HB3	1:A:146:VAL:HG12	0.52	1.82	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:196:TYR:N	1:A:225:ILE:O	0.52	2.43	9	2
1:A:173:VAL:CG1	1:A:197:LYS:O	0.52	2.58	7	1
1:A:176:LEU:CG	1:A:195:VAL:O	0.52	2.58	9	1
1:A:194:LEU:HD12	1:A:194:LEU:N	0.52	2.20	12	1
1:A:203:ARG:O	1:A:217:LEU:O	0.52	2.27	15	1
1:A:86:ILE:HG23	1:A:87:ARG:N	0.52	2.18	4	2
1:A:90:TYR:C	1:A:91:THR:OG1	0.52	2.52	10	2
1:A:134:ASN:O	1:A:138:ILE:CD1	0.52	2.58	13	1
1:A:192:LEU:CD1	1:A:229:CYS:O	0.51	2.58	7	2
1:A:203:ARG:NH2	1:A:205:ILE:HD13	0.51	2.19	1	1
1:A:141:LEU:O	1:A:142:VAL:CG2	0.51	2.58	3	1
1:A:100:ALA:O	1:A:102:PHE:CD1	0.51	2.63	4	1
1:A:123:TYR:CE1	1:A:198:PHE:CD2	0.51	2.98	1	1
1:A:90:TYR:CE1	1:A:92:PHE:CG	0.51	2.98	4	1
1:A:173:VAL:N	1:A:174:PRO:CD	0.51	2.73	8	2
1:A:173:VAL:HG13	1:A:199:ASP:CB	0.51	2.35	14	1
1:A:168:ILE:CB	1:A:201:LYS:O	0.51	2.58	5	5
1:A:170:PHE:O	1:A:171:ASN:C	0.51	2.53	8	13
1:A:144:LEU:O	1:A:148:GLU:CG	0.51	2.58	2	2
1:A:131:ALA:HB2	1:A:165:TRP:CG	0.51	2.40	3	1
1:A:157:LEU:CD2	1:A:159:GLY:N	0.51	2.73	5	1
1:A:192:LEU:CD2	1:A:194:LEU:HD23	0.51	2.36	14	1
1:A:138:ILE:HD11	1:A:147:GLN:HA	0.51	1.83	1	1
1:A:146:VAL:O	1:A:150:LEU:CB	0.51	2.59	15	2
1:A:147:GLN:NE2	1:A:151:GLU:OE1	0.51	2.44	9	1
1:A:196:TYR:O	1:A:225:ILE:N	0.51	2.43	5	3
1:A:194:LEU:N	1:A:194:LEU:HD12	0.51	2.21	5	1
1:A:150:LEU:C	1:A:150:LEU:HD13	0.51	2.31	9	1
1:A:126:VAL:CG1	1:A:238:LEU:CD1	0.51	2.88	15	1
1:A:191:HIS:CG	1:A:228:LEU:HD11	0.51	2.40	15	1
1:A:190:GLU:O	1:A:191:HIS:ND1	0.51	2.44	2	1
1:A:130:PHE:CE2	1:A:150:LEU:HD23	0.51	2.41	3	1
1:A:86:ILE:CG2	1:A:87:ARG:N	0.51	2.74	7	3
1:A:154:SER:O	1:A:157:LEU:CD2	0.51	2.58	11	2
1:A:147:GLN:O	1:A:151:GLU:N	0.51	2.44	9	2
1:A:192:LEU:HB3	1:A:194:LEU:HD11	0.51	1.83	15	1
1:A:102:PHE:C	1:A:102:PHE:CD2	0.51	2.88	2	1
1:A:91:THR:OG1	1:A:95:ASN:ND2	0.51	2.44	4	1
1:A:127:ASN:ND2	1:A:165:TRP:O	0.51	2.44	4	1
1:A:146:VAL:CG2	1:A:238:LEU:C	0.51	2.84	6	1
1:A:192:LEU:O	1:A:228:LEU:CB	0.51	2.58	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:VAL:HG23	1:A:100:ALA:N	0.51	2.19	8	3
1:A:155:ARG:O	1:A:157:LEU:CD1	0.51	2.58	2	1
1:A:226:ALA:O	1:A:239:MET:CB	0.51	2.58	15	4
1:A:198:PHE:CE2	1:A:200:THR:HB	0.51	2.41	9	3
1:A:228:LEU:HB2	1:A:237:ILE:CG1	0.51	2.35	12	1
1:A:204:LEU:O	1:A:204:LEU:HD12	0.51	2.06	15	1
1:A:204:LEU:O	1:A:205:ILE:CD1	0.51	2.59	15	1
1:A:206:LYS:HB2	1:A:215:GLU:N	0.51	2.21	15	1
1:A:163:LEU:HD23	1:A:206:LYS:HB2	0.51	1.83	1	1
1:A:229:CYS:SG	1:A:236:MET:CG	0.51	2.99	1	1
1:A:161:ALA:CB	1:A:207:VAL:O	0.51	2.58	3	1
1:A:174:PRO:HA	1:A:197:LYS:O	0.51	2.06	3	2
1:A:90:TYR:O	1:A:91:THR:CG2	0.51	2.59	4	2
1:A:198:PHE:CZ	1:A:200:THR:HB	0.51	2.41	15	3
1:A:157:LEU:HD12	1:A:159:GLY:N	0.51	2.20	7	1
1:A:176:LEU:HD11	1:A:196:TYR:CE2	0.51	2.39	12	1
1:A:88:ARG:O	1:A:92:PHE:CD1	0.51	2.63	2	1
1:A:175:LYS:N	1:A:197:LYS:O	0.51	2.43	9	4
1:A:198:PHE:CD1	1:A:225:ILE:HG13	0.51	2.41	5	1
1:A:159:GLY:O	1:A:161:ALA:N	0.51	2.44	15	1
1:A:146:VAL:CG2	1:A:239:MET:C	0.50	2.85	2	4
1:A:196:TYR:HE2	1:A:225:ILE:HG22	0.50	1.66	5	1
1:A:175:LYS:HG2	1:A:176:LEU:N	0.50	2.20	14	1
1:A:123:TYR:O	1:A:126:VAL:CG2	0.50	2.59	15	1
1:A:85:LEU:C	1:A:85:LEU:CD1	0.50	2.85	1	1
1:A:164:ASP:HB2	1:A:205:ILE:CG2	0.50	2.37	9	2
1:A:194:LEU:C	1:A:194:LEU:CD1	0.50	2.84	6	1
1:A:207:VAL:O	1:A:207:VAL:CG1	0.50	2.59	7	1
1:A:120:ILE:HG22	1:A:198:PHE:CD2	0.50	2.41	13	1
1:A:192:LEU:O	1:A:228:LEU:CD1	0.50	2.58	14	1
1:A:102:PHE:CD2	1:A:103:ARG:N	0.50	2.80	2	1
1:A:90:TYR:CE1	1:A:92:PHE:HB2	0.50	2.42	4	1
1:A:192:LEU:O	1:A:229:CYS:N	0.50	2.43	4	1
1:A:195:VAL:HG11	1:A:224:TYR:OH	0.50	2.05	6	1
1:A:141:LEU:O	1:A:142:VAL:CG1	0.50	2.58	12	2
1:A:196:TYR:CZ	1:A:225:ILE:HB	0.50	2.41	4	3
1:A:141:LEU:O	1:A:142:VAL:HG12	0.50	2.05	11	1
1:A:168:ILE:HB	1:A:201:LYS:O	0.50	2.07	15	9
1:A:193:GLN:HG2	1:A:228:LEU:HD11	0.50	1.83	12	1
1:A:85:LEU:O	1:A:88:ARG:CD	0.50	2.58	13	1
1:A:176:LEU:CD2	1:A:197:LYS:CG	0.50	2.90	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:SER:O	1:A:133:LYS:N	0.50	2.45	1	1
1:A:198:PHE:CE2	1:A:200:THR:OG1	0.50	2.63	1	1
1:A:141:LEU:C	1:A:142:VAL:HG22	0.50	2.31	3	1
1:A:165:TRP:CD2	1:A:165:TRP:O	0.50	2.65	5	1
1:A:135:LEU:O	1:A:138:ILE:CG2	0.50	2.59	15	1
1:A:130:PHE:HB3	1:A:165:TRP:CZ3	0.50	2.41	3	1
1:A:90:TYR:C	1:A:91:THR:CG2	0.50	2.85	4	1
1:A:222:VAL:O	1:A:222:VAL:CG2	0.50	2.59	12	5
1:A:228:LEU:CD2	1:A:239:MET:CG	0.50	2.90	9	1
1:A:194:LEU:O	1:A:226:ALA:CB	0.50	2.59	14	1
1:A:165:TRP:CE2	1:A:204:LEU:CD1	0.50	2.95	2	1
1:A:90:TYR:O	1:A:91:THR:C	0.50	2.54	4	5
1:A:204:LEU:N	1:A:217:LEU:O	0.50	2.44	7	4
1:A:146:VAL:CG2	1:A:238:LEU:O	0.50	2.60	7	2
1:A:132:HIS:NE2	1:A:164:ASP:OD2	0.50	2.44	14	1
1:A:203:ARG:CA	1:A:217:LEU:O	0.50	2.60	1	1
1:A:204:LEU:C	1:A:204:LEU:CD2	0.50	2.85	2	1
1:A:91:THR:O	1:A:93:GLY:N	0.50	2.44	5	1
1:A:95:ASN:O	1:A:98:GLN:N	0.50	2.44	10	1
1:A:167:LEU:CD1	1:A:200:THR:OG1	0.50	2.58	10	1
1:A:81:VAL:HG13	1:A:82:ALA:N	0.49	2.21	14	2
1:A:124:ILE:CG2	1:A:167:LEU:HD11	0.49	2.38	4	1
1:A:136:SER:O	1:A:139:LYS:N	0.49	2.44	7	2
1:A:155:ARG:HD3	1:A:156:GLN:N	0.49	2.22	8	1
1:A:163:LEU:HD11	1:A:206:LYS:HG3	0.49	1.83	12	1
1:A:130:PHE:CZ	1:A:150:LEU:HD12	0.49	2.42	4	1
1:A:150:LEU:O	1:A:154:SER:CB	0.49	2.60	5	1
1:A:198:PHE:CD1	1:A:198:PHE:O	0.49	2.66	7	1
1:A:228:LEU:CD2	1:A:239:MET:HG3	0.49	2.37	9	1
1:A:120:ILE:HB	1:A:198:PHE:CZ	0.49	2.42	13	1
1:A:223:ASP:C	1:A:224:TYR:CD1	0.49	2.91	2	4
1:A:135:LEU:HA	1:A:138:ILE:HD11	0.49	1.82	2	1
1:A:101:LEU:C	1:A:101:LEU:CD2	0.49	2.83	10	2
1:A:228:LEU:CD1	1:A:237:ILE:HG21	0.49	2.25	9	1
1:A:191:HIS:C	1:A:192:LEU:CD1	0.49	2.83	10	1
1:A:175:LYS:HG3	1:A:197:LYS:CB	0.49	2.37	7	1
1:A:230:ASP:N	1:A:235:ASP:OD1	0.49	2.44	13	2
1:A:117:ASN:O	1:A:121:GLU:N	0.49	2.45	14	1
1:A:217:LEU:C	1:A:217:LEU:CD2	0.49	2.85	1	1
1:A:195:VAL:HG11	1:A:224:TYR:CE1	0.49	2.42	6	1
1:A:146:VAL:CG1	1:A:150:LEU:HD12	0.49	2.35	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:LEU:O	1:A:226:ALA:HB1	0.49	2.07	14	1
1:A:203:ARG:NH2	1:A:205:ILE:CD1	0.49	2.76	1	1
1:A:190:GLU:O	1:A:190:GLU:CG	0.49	2.61	2	1
1:A:167:LEU:CD1	1:A:198:PHE:CZ	0.49	2.94	15	1
1:A:87:ARG:O	1:A:91:THR:CB	0.49	2.61	5	2
1:A:192:LEU:O	1:A:228:LEU:HA	0.49	2.07	6	7
1:A:242:LEU:CD2	1:A:243:PHE:HB2	0.49	2.38	2	1
1:A:223:ASP:C	1:A:224:TYR:CD2	0.49	2.91	13	3
1:A:167:LEU:CD1	1:A:200:THR:HG21	0.49	2.37	10	1
1:A:118:LYS:O	1:A:121:GLU:CB	0.49	2.60	13	2
1:A:117:ASN:O	1:A:121:GLU:CB	0.49	2.61	14	1
1:A:142:VAL:HG12	1:A:143:SER:N	0.49	2.23	14	4
1:A:98:GLN:OE1	1:A:194:LEU:CD2	0.49	2.61	2	1
1:A:157:LEU:N	1:A:157:LEU:HD13	0.49	2.22	5	1
1:A:150:LEU:C	1:A:150:LEU:CD1	0.49	2.85	9	1
1:A:169:LYS:NZ	1:A:171:ASN:OD1	0.49	2.44	9	1
1:A:168:ILE:HB	1:A:202:GLN:HB2	0.49	1.84	15	1
1:A:194:LEU:HB3	1:A:227:PHE:CD2	0.49	2.43	6	1
1:A:199:ASP:OD1	1:A:222:VAL:HG12	0.49	2.05	6	1
1:A:135:LEU:N	1:A:135:LEU:HD22	0.49	2.23	9	1
1:A:161:ALA:HB1	1:A:206:LYS:HD2	0.49	1.85	11	1
1:A:124:ILE:HG13	1:A:167:LEU:HD21	0.49	1.83	14	1
1:A:130:PHE:CE1	1:A:154:SER:HB3	0.49	2.43	15	1
1:A:172:ALA:O	1:A:173:VAL:C	0.48	2.55	9	7
1:A:176:LEU:HD13	1:A:196:TYR:CE2	0.48	2.43	1	1
1:A:196:TYR:C	1:A:224:TYR:CE1	0.48	2.91	4	1
1:A:228:LEU:CD1	1:A:239:MET:SD	0.48	3.01	10	1
1:A:166:GLN:C	1:A:167:LEU:HD12	0.48	2.32	11	1
1:A:227:PHE:CZ	1:A:238:LEU:CD1	0.48	2.95	1	1
1:A:161:ALA:HB1	1:A:206:LYS:HD3	0.48	1.85	5	1
1:A:132:HIS:C	1:A:133:LYS:CG	0.48	2.86	12	1
1:A:224:TYR:CD2	1:A:242:LEU:HB3	0.48	2.43	14	1
1:A:161:ALA:CB	1:A:207:VAL:HB	0.48	2.38	15	1
1:A:146:VAL:HG21	1:A:238:LEU:CD2	0.48	2.32	2	1
1:A:165:TRP:O	1:A:165:TRP:CE3	0.48	2.66	5	1
1:A:227:PHE:CZ	1:A:238:LEU:HG	0.48	2.42	7	1
1:A:135:LEU:N	1:A:135:LEU:CD2	0.48	2.76	9	1
1:A:88:ARG:CA	1:A:91:THR:HG23	0.48	2.34	12	1
1:A:199:ASP:OD1	1:A:222:VAL:CG2	0.48	2.58	14	1
1:A:155:ARG:O	1:A:156:GLN:C	0.48	2.57	9	14
1:A:242:LEU:HD22	1:A:242:LEU:O	0.48	2.07	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:LEU:HD22	1:A:177:VAL:HG13	0.48	1.85	12	1
1:A:91:THR:O	1:A:95:ASN:CB	0.48	2.61	13	1
1:A:161:ALA:HB1	1:A:207:VAL:HB	0.48	1.85	15	1
1:A:242:LEU:HD22	1:A:243:PHE:HB2	0.48	1.85	2	1
1:A:98:GLN:O	1:A:101:LEU:HD23	0.48	2.07	4	1
1:A:130:PHE:CZ	1:A:150:LEU:CD1	0.48	2.97	4	1
1:A:164:ASP:HB3	1:A:205:ILE:HD11	0.48	1.85	14	2
1:A:228:LEU:HD22	1:A:239:MET:SD	0.48	2.48	6	1
1:A:167:LEU:CD2	1:A:200:THR:CG2	0.48	2.88	10	1
1:A:142:VAL:O	1:A:142:VAL:CG1	0.48	2.61	11	1
1:A:176:LEU:CD1	1:A:196:TYR:CE2	0.48	2.96	12	1
1:A:101:LEU:HD13	1:A:101:LEU:C	0.48	2.30	14	1
1:A:146:VAL:CG1	1:A:147:GLN:N	0.48	2.76	1	2
1:A:146:VAL:O	1:A:150:LEU:N	0.48	2.47	3	1
1:A:177:VAL:O	1:A:195:VAL:HG12	0.48	2.08	6	1
1:A:192:LEU:CD1	1:A:192:LEU:N	0.48	2.77	10	1
1:A:154:SER:O	1:A:157:LEU:CD1	0.48	2.61	14	2
1:A:162:THR:OG1	1:A:207:VAL:CG1	0.48	2.61	7	1
1:A:203:ARG:HG2	1:A:218:ASP:CA	0.48	2.39	8	1
1:A:172:ALA:CB	1:A:199:ASP:CG	0.48	2.87	15	1
1:A:205:ILE:O	1:A:205:ILE:CG2	0.48	2.60	1	3
1:A:197:LYS:HG3	1:A:224:TYR:CE2	0.48	2.43	3	1
1:A:205:ILE:CG1	1:A:205:ILE:O	0.48	2.62	11	3
1:A:141:LEU:N	1:A:141:LEU:HD12	0.48	2.23	10	2
1:A:141:LEU:CD1	1:A:141:LEU:N	0.48	2.76	11	1
1:A:141:LEU:O	1:A:143:SER:N	0.48	2.47	7	4
1:A:167:LEU:CA	1:A:202:GLN:HB3	0.48	2.39	15	1
1:A:122:THR:O	1:A:126:VAL:N	0.48	2.46	2	1
1:A:102:PHE:CE1	1:A:103:ARG:HG3	0.48	2.42	5	1
1:A:162:THR:HB	1:A:207:VAL:CG1	0.48	2.39	7	1
1:A:225:ILE:HD11	1:A:238:LEU:HG	0.48	1.84	14	1
1:A:85:LEU:O	1:A:89:LEU:CB	0.47	2.62	8	2
1:A:141:LEU:O	1:A:142:VAL:C	0.47	2.57	3	1
1:A:125:ASN:O	1:A:128:THR:N	0.47	2.47	10	1
1:A:91:THR:OG1	1:A:95:ASN:CB	0.47	2.61	12	1
1:A:95:ASN:O	1:A:99:VAL:HG23	0.47	2.09	12	1
1:A:95:ASN:OD1	1:A:99:VAL:CG2	0.47	2.61	15	1
1:A:95:ASN:O	1:A:99:VAL:HG22	0.47	2.09	7	2
1:A:176:LEU:HD23	1:A:195:VAL:O	0.47	2.09	6	2
1:A:172:ALA:C	1:A:199:ASP:CB	0.47	2.87	7	1
1:A:204:LEU:CB	1:A:217:LEU:HB3	0.47	2.39	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:ILE:HG12	1:A:143:SER:CB	0.47	2.39	12	1
1:A:134:ASN:OD1	1:A:137:ASP:CB	0.47	2.62	1	1
1:A:222:VAL:O	1:A:222:VAL:CG1	0.47	2.62	7	3
1:A:86:ILE:O	1:A:89:LEU:CB	0.47	2.63	4	1
1:A:197:LYS:HB2	1:A:224:TYR:CE2	0.47	2.43	4	1
1:A:175:LYS:C	1:A:176:LEU:HG	0.47	2.34	6	3
1:A:190:GLU:O	1:A:230:ASP:CG	0.47	2.58	6	3
1:A:162:THR:CB	1:A:207:VAL:CG1	0.47	2.92	7	1
1:A:172:ALA:O	1:A:173:VAL:CB	0.47	2.62	15	3
1:A:126:VAL:HG11	1:A:238:LEU:CD2	0.47	2.40	3	1
1:A:204:LEU:CB	1:A:217:LEU:HB2	0.47	2.38	4	1
1:A:142:VAL:HG12	1:A:147:GLN:N	0.47	2.24	8	1
1:A:166:GLN:CG	1:A:203:ARG:O	0.47	2.62	8	1
1:A:194:LEU:HB3	1:A:196:TYR:CE1	0.47	2.45	1	1
1:A:119:ALA:HB3	1:A:196:TYR:CG	0.47	2.45	7	1
1:A:88:ARG:HG3	1:A:92:PHE:CD2	0.47	2.45	11	1
1:A:120:ILE:CB	1:A:198:PHE:CE2	0.47	2.97	13	1
1:A:100:ALA:O	1:A:101:LEU:C	0.47	2.56	10	4
1:A:138:ILE:HD11	1:A:147:GLN:OE1	0.47	2.09	6	1
1:A:143:SER:CB	1:A:237:ILE:CG2	0.47	2.93	8	1
1:A:173:VAL:HG22	1:A:199:ASP:HB3	0.47	1.85	14	1
1:A:143:SER:CB	1:A:146:VAL:CG1	0.47	2.93	9	2
1:A:95:ASN:O	1:A:96:SER:C	0.47	2.58	2	5
1:A:92:PHE:O	1:A:96:SER:N	0.47	2.45	7	3
1:A:227:PHE:CE2	1:A:238:LEU:HG	0.47	2.45	7	1
1:A:163:LEU:HD21	1:A:206:LYS:CG	0.47	2.39	9	1
1:A:228:LEU:O	1:A:237:ILE:CB	0.47	2.63	11	1
1:A:123:TYR:O	1:A:126:VAL:HG22	0.47	2.09	15	2
1:A:175:LYS:HD2	1:A:197:LYS:CB	0.47	2.39	13	1
1:A:130:PHE:HB3	1:A:165:TRP:CD1	0.47	2.45	14	1
1:A:201:LYS:CD	1:A:219:ARG:O	0.47	2.62	14	1
1:A:160:ASN:O	1:A:208:ASN:O	0.47	2.33	15	1
1:A:203:ARG:CG	1:A:217:LEU:C	0.47	2.87	2	1
1:A:168:ILE:O	1:A:200:THR:OG1	0.47	2.30	10	4
1:A:167:LEU:HD21	1:A:200:THR:CB	0.47	2.39	5	1
1:A:173:VAL:N	1:A:174:PRO:HD3	0.47	2.25	8	2
1:A:163:LEU:HD21	1:A:206:LYS:HG3	0.47	1.87	9	1
1:A:161:ALA:HB1	1:A:207:VAL:CG1	0.47	2.40	15	1
1:A:227:PHE:CZ	1:A:238:LEU:HD13	0.47	2.45	1	1
1:A:93:GLY:O	1:A:97:VAL:CG2	0.47	2.61	4	1
1:A:168:ILE:HD11	1:A:203:ARG:HB2	0.47	1.85	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:224:TYR:O	1:A:241:SER:HB2	0.47	2.10	6	11
1:A:225:ILE:CG1	1:A:241:SER:HB3	0.47	2.40	15	4
1:A:100:ALA:HA	1:A:102:PHE:CD1	0.47	2.45	4	1
1:A:131:ALA:CB	1:A:164:ASP:HA	0.47	2.39	6	1
1:A:173:VAL:HG11	1:A:197:LYS:C	0.47	2.34	7	1
1:A:192:LEU:O	1:A:227:PHE:O	0.47	2.34	8	1
1:A:176:LEU:HD21	1:A:196:TYR:CG	0.47	2.45	12	1
1:A:124:ILE:HD12	1:A:167:LEU:CD2	0.47	2.39	15	1
1:A:228:LEU:CD2	1:A:237:ILE:HB	0.47	2.40	15	1
1:A:171:ASN:O	1:A:172:ALA:CB	0.46	2.57	9	3
1:A:127:ASN:O	1:A:128:THR:C	0.46	2.59	2	5
1:A:132:HIS:O	1:A:132:HIS:CG	0.46	2.66	7	1
1:A:230:ASP:OD2	1:A:230:ASP:N	0.46	2.47	7	1
1:A:91:THR:OG1	1:A:95:ASN:CG	0.46	2.57	10	1
1:A:227:PHE:CD2	1:A:227:PHE:C	0.46	2.91	12	1
1:A:144:LEU:CD1	1:A:145:TRP:CD1	0.46	2.97	14	1
1:A:204:LEU:C	1:A:205:ILE:CD1	0.46	2.82	15	1
1:A:169:LYS:HA	1:A:200:THR:HG22	0.46	1.86	8	3
1:A:147:GLN:CG	1:A:151:GLU:CD	0.46	2.89	5	1
1:A:78:PRO:O	1:A:81:VAL:CG2	0.46	2.58	12	1
1:A:167:LEU:HD12	1:A:198:PHE:HZ	0.46	1.66	15	1
1:A:168:ILE:CG1	1:A:202:GLN:HB2	0.46	2.40	15	1
1:A:135:LEU:C	1:A:135:LEU:CD2	0.46	2.88	3	1
1:A:98:GLN:O	1:A:101:LEU:CG	0.46	2.63	4	1
1:A:117:ASN:O	1:A:118:LYS:C	0.46	2.58	4	4
1:A:198:PHE:CE1	1:A:225:ILE:CG1	0.46	2.99	5	1
1:A:227:PHE:CE1	1:A:238:LEU:HG	0.46	2.45	11	1
1:A:124:ILE:HG23	1:A:125:ASN:N	0.46	2.24	14	1
1:A:80:ILE:HG23	1:A:81:VAL:N	0.46	2.26	15	1
1:A:203:ARG:HB3	1:A:217:LEU:O	0.46	2.11	15	1
1:A:156:GLN:O	1:A:157:LEU:O	0.46	2.33	6	12
1:A:119:ALA:HB1	1:A:227:PHE:CE1	0.46	2.46	2	1
1:A:153:ARG:O	1:A:154:SER:C	0.46	2.58	2	3
1:A:129:SER:CB	1:A:134:ASN:OD1	0.46	2.63	6	1
1:A:205:ILE:O	1:A:205:ILE:HD12	0.46	2.11	11	3
1:A:89:LEU:C	1:A:89:LEU:CD2	0.46	2.87	8	1
1:A:91:THR:O	1:A:92:PHE:CB	0.46	2.64	10	1
1:A:228:LEU:HB2	1:A:237:ILE:CD1	0.46	2.40	12	1
1:A:122:THR:CG2	1:A:141:LEU:HD12	0.46	2.37	2	1
1:A:146:VAL:O	1:A:147:GLN:C	0.46	2.58	11	4
1:A:194:LEU:HD13	1:A:194:LEU:C	0.46	2.34	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:PHE:O	1:A:131:ALA:C	0.46	2.58	7	2
1:A:143:SER:HB2	1:A:237:ILE:CG2	0.46	2.41	8	2
1:A:199:ASP:C	1:A:200:THR:HG23	0.46	2.34	2	2
1:A:155:ARG:O	1:A:157:LEU:N	0.46	2.43	5	1
1:A:226:ALA:O	1:A:239:MET:O	0.46	2.33	10	2
1:A:203:ARG:CG	1:A:218:ASP:CB	0.46	2.93	8	1
1:A:230:ASP:O	1:A:230:ASP:CG	0.46	2.57	8	1
1:A:94:LEU:C	1:A:94:LEU:CD1	0.46	2.88	10	2
1:A:146:VAL:HG13	1:A:239:MET:HG2	0.46	1.86	10	1
1:A:96:SER:O	1:A:100:ALA:N	0.46	2.48	13	1
1:A:120:ILE:HB	1:A:198:PHE:CE2	0.46	2.45	13	1
1:A:122:THR:O	1:A:123:TYR:C	0.46	2.58	9	9
1:A:129:SER:O	1:A:133:LYS:C	0.46	2.59	1	1
1:A:172:ALA:O	1:A:199:ASP:CG	0.46	2.58	7	1
1:A:204:LEU:HB3	1:A:217:LEU:CB	0.46	2.40	7	2
1:A:205:ILE:O	1:A:205:ILE:CG1	0.46	2.63	7	1
1:A:139:LYS:O	1:A:140:GLY:C	0.46	2.57	9	2
1:A:242:LEU:O	1:A:243:PHE:O	0.46	2.34	2	1
1:A:87:ARG:O	1:A:91:THR:OG1	0.46	2.34	5	1
1:A:118:LYS:O	1:A:119:ALA:C	0.46	2.58	9	4
1:A:79:LEU:O	1:A:79:LEU:CD1	0.46	2.64	6	1
1:A:196:TYR:CE1	1:A:197:LYS:C	0.46	2.94	7	1
1:A:127:ASN:O	1:A:130:PHE:N	0.46	2.47	9	1
1:A:199:ASP:OD2	1:A:221:VAL:O	0.46	2.34	10	1
1:A:174:PRO:O	1:A:175:LYS:CB	0.46	2.59	14	3
1:A:236:MET:SD	1:A:236:MET:O	0.46	2.73	12	1
1:A:147:GLN:CG	1:A:148:GLU:N	0.46	2.78	13	1
1:A:168:ILE:O	1:A:201:LYS:N	0.46	2.47	15	1
1:A:204:LEU:O	1:A:205:ILE:CG1	0.46	2.64	15	1
1:A:88:ARG:O	1:A:89:LEU:C	0.46	2.58	2	3
1:A:203:ARG:HG3	1:A:217:LEU:C	0.46	2.36	2	2
1:A:149:ALA:O	1:A:152:ALA:HB3	0.46	2.11	5	3
1:A:230:ASP:N	1:A:235:ASP:OD2	0.46	2.48	3	1
1:A:224:TYR:C	1:A:225:ILE:CD1	0.46	2.82	6	1
1:A:157:LEU:HD12	1:A:158:PRO:N	0.46	2.26	8	2
1:A:169:LYS:HA	1:A:200:THR:OG1	0.46	2.11	9	1
1:A:192:LEU:O	1:A:228:LEU:CG	0.46	2.64	12	1
1:A:205:ILE:HG22	1:A:216:THR:HA	0.46	1.88	13	1
1:A:222:VAL:HG22	1:A:224:TYR:CE1	0.46	2.46	2	1
1:A:123:TYR:OH	1:A:198:PHE:CE2	0.46	2.66	5	1
1:A:196:TYR:O	1:A:224:TYR:HA	0.45	2.10	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:ARG:HA	1:A:217:LEU:O	0.45	2.11	1	10
1:A:222:VAL:HG22	1:A:224:TYR:HE1	0.45	1.70	2	1
1:A:92:PHE:HB3	1:A:95:ASN:CB	0.45	2.41	11	3
1:A:225:ILE:HA	1:A:241:SER:CB	0.45	2.41	9	6
1:A:132:HIS:CD2	1:A:132:HIS:N	0.45	2.84	7	1
1:A:159:GLY:O	1:A:160:ASN:OD1	0.45	2.34	9	2
1:A:141:LEU:N	1:A:141:LEU:CD1	0.45	2.80	14	1
1:A:94:LEU:N	1:A:94:LEU:HD22	0.45	2.26	15	1
1:A:177:VAL:O	1:A:177:VAL:CG1	0.45	2.64	15	1
1:A:173:VAL:CG1	1:A:174:PRO:HD2	0.45	2.41	4	4
1:A:92:PHE:CE1	1:A:96:SER:HB2	0.45	2.46	8	1
1:A:167:LEU:CD1	1:A:200:THR:CG2	0.45	2.92	10	1
1:A:235:ASP:OD2	1:A:235:ASP:O	0.45	2.34	13	1
1:A:175:LYS:HG2	1:A:176:LEU:H	0.45	1.70	14	1
1:A:164:ASP:O	1:A:165:TRP:O	0.45	2.35	15	1
1:A:203:ARG:CG	1:A:217:LEU:O	0.45	2.65	2	1
1:A:142:VAL:O	1:A:142:VAL:HG12	0.45	2.12	6	2
1:A:173:VAL:N	1:A:199:ASP:HB2	0.45	2.26	7	1
1:A:95:ASN:ND2	1:A:99:VAL:HG11	0.45	2.27	8	1
1:A:128:THR:HA	1:A:165:TRP:CD2	0.45	2.47	11	1
1:A:93:GLY:O	1:A:94:LEU:C	0.45	2.58	12	1
1:A:89:LEU:O	1:A:90:TYR:C	0.45	2.59	13	1
1:A:88:ARG:HA	1:A:91:THR:CG2	0.45	2.41	15	1
1:A:96:SER:O	1:A:100:ALA:CB	0.45	2.64	8	2
1:A:95:ASN:ND2	1:A:99:VAL:CG2	0.45	2.80	4	1
1:A:102:PHE:O	1:A:103:ARG:C	0.45	2.59	6	3
1:A:201:LYS:HE3	1:A:219:ARG:C	0.45	2.36	6	1
1:A:206:LYS:O	1:A:213:LYS:O	0.45	2.34	7	3
1:A:95:ASN:ND2	1:A:99:VAL:CG1	0.45	2.79	7	2
1:A:120:ILE:O	1:A:121:GLU:C	0.45	2.60	11	2
1:A:197:LYS:CE	1:A:224:TYR:CE2	0.45	2.99	7	1
1:A:95:ASN:OD1	1:A:98:GLN:OE1	0.45	2.35	8	1
1:A:135:LEU:HD21	1:A:151:GLU:OE2	0.45	2.12	8	1
1:A:229:CYS:CB	1:A:235:ASP:O	0.45	2.64	8	2
1:A:91:THR:HG21	1:A:94:LEU:HD11	0.45	1.86	10	1
1:A:91:THR:O	1:A:92:PHE:CG	0.45	2.70	1	1
1:A:129:SER:CB	1:A:134:ASN:HB3	0.45	2.41	15	3
1:A:204:LEU:HB2	1:A:217:LEU:CB	0.45	2.42	4	1
1:A:230:ASP:O	1:A:230:ASP:OD2	0.45	2.34	5	2
1:A:203:ARG:CG	1:A:218:ASP:HB2	0.45	2.42	8	1
1:A:99:VAL:CG1	1:A:100:ALA:N	0.45	2.80	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:225:ILE:HG23	1:A:241:SER:HB3	0.45	1.87	9	2
1:A:176:LEU:O	1:A:195:VAL:O	0.45	2.35	11	1
1:A:136:SER:O	1:A:137:ASP:C	0.45	2.59	6	6
1:A:91:THR:O	1:A:92:PHE:O	0.45	2.34	4	3
1:A:91:THR:CA	1:A:95:ASN:HB3	0.45	2.41	4	1
1:A:96:SER:O	1:A:97:VAL:C	0.45	2.60	9	3
1:A:154:SER:O	1:A:155:ARG:C	0.45	2.59	7	3
1:A:173:VAL:HG22	1:A:197:LYS:HB3	0.45	1.88	7	1
1:A:222:VAL:HG22	1:A:224:TYR:HE2	0.45	1.71	7	1
1:A:229:CYS:HB2	1:A:235:ASP:O	0.45	2.11	8	1
1:A:208:ASN:O	1:A:208:ASN:CG	0.45	2.59	15	1
1:A:124:ILE:HD11	1:A:169:LYS:HE3	0.45	1.88	1	1
1:A:225:ILE:CG2	1:A:227:PHE:CE1	0.45	3.00	1	1
1:A:116:LYS:N	1:A:116:LYS:HD2	0.45	2.26	3	1
1:A:129:SER:O	1:A:133:LYS:O	0.45	2.35	12	2
1:A:156:GLN:NE2	1:A:156:GLN:N	0.45	2.64	3	1
1:A:197:LYS:HB2	1:A:224:TYR:CZ	0.45	2.46	4	1
1:A:85:LEU:C	1:A:85:LEU:CD2	0.45	2.89	5	3
1:A:116:LYS:CG	1:A:117:ASN:N	0.45	2.79	5	1
1:A:164:ASP:HB2	1:A:205:ILE:CD1	0.45	2.41	7	1
1:A:173:VAL:CG2	1:A:197:LYS:HB3	0.45	2.41	7	1
1:A:176:LEU:HD21	1:A:196:TYR:CD1	0.45	2.46	12	1
1:A:91:THR:O	1:A:91:THR:HG23	0.45	2.12	3	2
1:A:147:GLN:O	1:A:148:GLU:C	0.45	2.59	9	2
1:A:136:SER:O	1:A:139:LYS:CG	0.45	2.65	6	1
1:A:172:ALA:O	1:A:199:ASP:OD1	0.45	2.35	7	1
1:A:163:LEU:HD11	1:A:206:LYS:HB2	0.45	1.89	9	1
1:A:230:ASP:OD1	1:A:235:ASP:CG	0.45	2.59	15	1
1:A:147:GLN:O	1:A:151:GLU:HB3	0.45	2.12	2	7
1:A:230:ASP:OD2	1:A:230:ASP:C	0.45	2.58	2	1
1:A:143:SER:O	1:A:147:GLN:HB3	0.45	2.12	6	4
1:A:143:SER:O	1:A:147:GLN:HB2	0.45	2.12	12	2
1:A:241:SER:O	1:A:242:LEU:CD2	0.45	2.64	10	1
1:A:84:ALA:CB	1:A:88:ARG:NH1	0.45	2.79	11	1
1:A:158:PRO:O	1:A:159:GLY:C	0.45	2.59	15	1
1:A:164:ASP:O	1:A:165:TRP:C	0.45	2.58	15	1
1:A:167:LEU:N	1:A:202:GLN:HG2	0.45	2.27	15	1
1:A:172:ALA:C	1:A:173:VAL:CG2	0.45	2.90	15	1
1:A:229:CYS:SG	1:A:235:ASP:O	0.45	2.75	2	3
1:A:162:THR:HB	1:A:207:VAL:HG22	0.45	1.88	5	1
1:A:92:PHE:CZ	1:A:96:SER:HA	0.45	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:ILE:CG2	1:A:142:VAL:HG21	0.45	2.41	8	1
1:A:91:THR:O	1:A:95:ASN:HB3	0.45	2.12	13	1
1:A:168:ILE:HD12	1:A:202:GLN:NE2	0.45	2.27	15	1
1:A:230:ASP:CG	1:A:235:ASP:OD1	0.45	2.59	15	1
1:A:126:VAL:CG2	1:A:127:ASN:N	0.44	2.80	1	1
1:A:173:VAL:CG2	1:A:174:PRO:HD2	0.44	2.41	3	2
1:A:225:ILE:HG21	1:A:227:PHE:CZ	0.44	2.47	3	1
1:A:126:VAL:HG22	1:A:141:LEU:CD1	0.44	2.39	6	1
1:A:120:ILE:HG23	1:A:121:GLU:N	0.44	2.26	10	1
1:A:143:SER:HB3	1:A:146:VAL:CG2	0.44	2.42	10	1
1:A:167:LEU:HD13	1:A:167:LEU:C	0.44	2.37	10	1
1:A:235:ASP:OD1	1:A:235:ASP:O	0.44	2.34	15	1
1:A:82:ALA:O	1:A:83:ASN:C	0.44	2.59	4	3
1:A:138:ILE:O	1:A:142:VAL:N	0.44	2.48	8	2
1:A:198:PHE:CD1	1:A:225:ILE:HD12	0.44	2.46	5	1
1:A:138:ILE:CG2	1:A:139:LYS:N	0.44	2.79	9	2
1:A:118:LYS:O	1:A:121:GLU:N	0.44	2.50	9	2
1:A:150:LEU:C	1:A:150:LEU:CD2	0.44	2.83	11	1
1:A:197:LYS:HG2	1:A:224:TYR:CE2	0.44	2.47	12	1
1:A:90:TYR:O	1:A:91:THR:OG1	0.44	2.35	6	2
1:A:123:TYR:HA	1:A:126:VAL:CG2	0.44	2.42	10	2
1:A:226:ALA:CB	1:A:239:MET:O	0.44	2.56	10	1
1:A:94:LEU:O	1:A:95:ASN:C	0.44	2.60	11	1
1:A:237:ILE:C	1:A:237:ILE:CD1	0.44	2.81	12	1
1:A:230:ASP:O	1:A:235:ASP:OD1	0.44	2.34	13	1
1:A:174:PRO:HG2	1:A:197:LYS:CE	0.44	2.42	2	1
1:A:96:SER:O	1:A:100:ALA:HB3	0.44	2.12	8	1
1:A:138:ILE:HG13	1:A:143:SER:CB	0.44	2.43	9	1
1:A:163:LEU:CD2	1:A:206:LYS:HG3	0.44	2.43	9	1
1:A:171:ASN:O	1:A:172:ALA:O	0.44	2.36	14	1
1:A:228:LEU:CD2	1:A:237:ILE:HG13	0.44	2.43	15	1
1:A:177:VAL:C	1:A:195:VAL:CG1	0.44	2.90	1	1
1:A:99:VAL:CG2	1:A:100:ALA:N	0.44	2.80	2	2
1:A:228:LEU:CB	1:A:237:ILE:HB	0.44	2.43	5	6
1:A:227:PHE:CE1	1:A:236:MET:HB2	0.44	2.48	5	1
1:A:124:ILE:HG13	1:A:125:ASN:N	0.44	2.28	9	2
1:A:164:ASP:HB2	1:A:205:ILE:HG23	0.44	1.88	9	1
1:A:125:ASN:O	1:A:126:VAL:C	0.44	2.59	10	2
1:A:227:PHE:O	1:A:227:PHE:CD1	0.44	2.71	10	1
1:A:144:LEU:C	1:A:144:LEU:CD1	0.44	2.87	13	1
1:A:126:VAL:O	1:A:130:PHE:CD1	0.44	2.71	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:GLU:O	1:A:124:ILE:HG22	0.44	2.12	5	1
1:A:92:PHE:CE2	1:A:96:SER:HA	0.44	2.48	8	1
1:A:142:VAL:HG12	1:A:238:LEU:HD13	0.44	1.88	2	1
1:A:126:VAL:HG21	1:A:238:LEU:HD22	0.44	1.90	5	2
1:A:157:LEU:CD1	1:A:158:PRO:HD2	0.44	2.43	11	2
1:A:170:PHE:O	1:A:171:ASN:CB	0.44	2.63	7	1
1:A:148:GLU:O	1:A:152:ALA:HB3	0.44	2.13	9	1
1:A:197:LYS:HD3	1:A:198:PHE:N	0.44	2.27	11	1
1:A:204:LEU:H	1:A:205:ILE:HD12	0.44	1.72	15	1
1:A:157:LEU:HD13	1:A:158:PRO:HD2	0.44	1.89	6	1
1:A:136:SER:O	1:A:140:GLY:N	0.44	2.51	12	1
1:A:208:ASN:O	1:A:208:ASN:OD1	0.44	2.35	15	1
1:A:174:PRO:HB3	1:A:197:LYS:O	0.44	2.12	5	1
1:A:192:LEU:HB2	1:A:229:CYS:CB	0.44	2.42	6	1
1:A:147:GLN:HG3	1:A:151:GLU:CB	0.44	2.42	9	1
1:A:228:LEU:HD22	1:A:239:MET:HG3	0.44	1.89	9	1
1:A:222:VAL:O	1:A:223:ASP:OD2	0.44	2.36	10	1
1:A:194:LEU:O	1:A:226:ALA:CA	0.44	2.65	14	1
1:A:201:LYS:HD3	1:A:219:ARG:O	0.44	2.13	14	1
1:A:146:VAL:HG21	1:A:238:LEU:C	0.43	2.38	6	1
1:A:79:LEU:CD1	1:A:79:LEU:H	0.43	2.26	12	1
1:A:137:ASP:O	1:A:138:ILE:C	0.43	2.61	12	1
1:A:228:LEU:HB3	1:A:237:ILE:CD1	0.43	2.42	13	1
1:A:221:VAL:HG12	1:A:223:ASP:OD2	0.43	2.12	15	1
1:A:92:PHE:O	1:A:93:GLY:C	0.43	2.61	7	3
1:A:206:LYS:HB2	1:A:215:GLU:CB	0.43	2.42	15	1
1:A:228:LEU:CD2	1:A:237:ILE:CB	0.43	2.95	15	1
1:A:127:ASN:HA	1:A:130:PHE:CB	0.43	2.44	2	1
1:A:157:LEU:C	1:A:157:LEU:HD13	0.43	2.37	2	1
1:A:224:TYR:HB2	1:A:242:LEU:CD1	0.43	2.43	2	2
1:A:89:LEU:O	1:A:89:LEU:HD13	0.43	2.12	6	1
1:A:229:CYS:HA	1:A:235:ASP:O	0.43	2.12	6	1
1:A:92:PHE:O	1:A:96:SER:HB2	0.43	2.12	8	2
1:A:222:VAL:C	1:A:223:ASP:CG	0.43	2.87	10	1
1:A:98:GLN:OE1	1:A:98:GLN:O	0.43	2.36	12	1
1:A:134:ASN:ND2	1:A:137:ASP:OD2	0.43	2.51	12	1
1:A:227:PHE:CD1	1:A:236:MET:HB3	0.43	2.48	14	1
1:A:101:LEU:O	1:A:102:PHE:C	0.43	2.58	4	2
1:A:157:LEU:CD1	1:A:159:GLY:N	0.43	2.81	7	1
1:A:193:GLN:HG2	1:A:228:LEU:CD1	0.43	2.43	12	1
1:A:119:ALA:CB	1:A:196:TYR:CD2	0.43	3.01	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:LEU:HA	1:A:88:ARG:NE	0.43	2.28	2	1
1:A:199:ASP:CB	1:A:222:VAL:HG12	0.43	2.41	6	1
1:A:121:GLU:O	1:A:124:ILE:HG13	0.43	2.14	4	1
1:A:116:LYS:HG3	1:A:117:ASN:N	0.43	2.28	5	2
1:A:196:TYR:C	1:A:196:TYR:CD2	0.43	2.96	6	1
1:A:197:LYS:HE2	1:A:224:TYR:CE2	0.43	2.49	7	1
1:A:163:LEU:CD1	1:A:206:LYS:HB2	0.43	2.44	9	1
1:A:196:TYR:CD2	1:A:198:PHE:CE2	0.43	3.06	10	1
1:A:138:ILE:HG13	1:A:143:SER:OG	0.43	2.14	12	1
1:A:87:ARG:O	1:A:88:ARG:C	0.43	2.61	13	1
1:A:208:ASN:OD1	1:A:208:ASN:N	0.43	2.50	1	1
1:A:235:ASP:OD1	1:A:235:ASP:N	0.43	2.51	2	1
1:A:225:ILE:HA	1:A:241:SER:HB2	0.43	1.90	13	2
1:A:176:LEU:C	1:A:176:LEU:CD2	0.43	2.88	5	1
1:A:78:PRO:O	1:A:79:LEU:C	0.43	2.60	10	1
1:A:81:VAL:CG2	1:A:82:ALA:N	0.43	2.81	10	1
1:A:175:LYS:O	1:A:176:LEU:HG	0.43	2.14	10	1
1:A:142:VAL:HG23	1:A:143:SER:H	0.43	1.72	12	1
1:A:213:LYS:HG2	1:A:214:THR:N	0.43	2.29	14	1
1:A:123:TYR:HE1	1:A:225:ILE:HD13	0.43	1.71	15	1
1:A:226:ALA:O	1:A:239:MET:HB2	0.43	2.13	15	1
1:A:171:ASN:OD1	1:A:171:ASN:N	0.43	2.52	1	1
1:A:129:SER:CB	1:A:134:ASN:HB2	0.43	2.44	2	1
1:A:156:GLN:O	1:A:157:LEU:C	0.43	2.59	2	1
1:A:132:HIS:O	1:A:133:LYS:O	0.43	2.35	3	1
1:A:100:ALA:HA	1:A:102:PHE:CE1	0.43	2.49	4	1
1:A:150:LEU:O	1:A:154:SER:HB3	0.43	2.14	5	1
1:A:146:VAL:CG2	1:A:239:MET:O	0.43	2.66	6	1
1:A:119:ALA:CB	1:A:196:TYR:CG	0.43	3.02	7	1
1:A:172:ALA:C	1:A:199:ASP:CG	0.43	2.87	7	1
1:A:227:PHE:HA	1:A:237:ILE:O	0.43	2.14	10	3
1:A:92:PHE:CB	1:A:95:ASN:HB3	0.43	2.44	9	1
1:A:92:PHE:CD2	1:A:92:PHE:C	0.43	2.97	13	1
1:A:87:ARG:O	1:A:91:THR:HB	0.43	2.14	5	2
1:A:92:PHE:CE2	1:A:95:ASN:CB	0.43	3.02	2	1
1:A:146:VAL:O	1:A:150:LEU:HB3	0.43	2.13	2	1
1:A:172:ALA:O	1:A:173:VAL:HB	0.43	2.13	2	3
1:A:198:PHE:CZ	1:A:200:THR:OG1	0.43	2.58	2	1
1:A:203:ARG:HG2	1:A:217:LEU:O	0.43	2.13	2	1
1:A:163:LEU:CD1	1:A:204:LEU:HD21	0.43	2.44	8	1
1:A:135:LEU:O	1:A:136:SER:C	0.43	2.60	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:PHE:CD1	1:A:165:TRP:NE1	0.43	2.87	14	1
1:A:173:VAL:HG13	1:A:199:ASP:CG	0.43	2.39	14	1
1:A:122:THR:O	1:A:125:ASN:N	0.43	2.45	15	1
1:A:168:ILE:O	1:A:200:THR:HG23	0.43	2.14	15	1
1:A:91:THR:HA	1:A:95:ASN:CB	0.43	2.44	4	1
1:A:138:ILE:HD11	1:A:147:GLN:CG	0.43	2.41	7	1
1:A:162:THR:C	1:A:163:LEU:HD22	0.43	2.39	9	1
1:A:101:LEU:C	1:A:101:LEU:CD1	0.42	2.87	4	2
1:A:136:SER:O	1:A:139:LYS:HG2	0.42	2.14	6	1
1:A:143:SER:OG	1:A:237:ILE:HG21	0.42	2.13	8	1
1:A:128:THR:HG23	1:A:165:TRP:NE1	0.42	2.28	10	1
1:A:132:HIS:C	1:A:133:LYS:HG3	0.42	2.38	12	1
1:A:142:VAL:O	1:A:143:SER:C	0.42	2.61	14	1
1:A:88:ARG:HA	1:A:91:THR:HG22	0.42	1.91	15	1
1:A:92:PHE:O	1:A:92:PHE:CD1	0.42	2.73	2	1
1:A:198:PHE:CE2	1:A:200:THR:HG21	0.42	2.50	2	1
1:A:196:TYR:CD1	1:A:197:LYS:N	0.42	2.88	7	1
1:A:163:LEU:CD1	1:A:206:LYS:CE	0.42	2.97	8	1
1:A:164:ASP:HB3	1:A:205:ILE:HG22	0.42	1.90	9	1
1:A:175:LYS:HE3	1:A:197:LYS:O	0.42	2.14	13	2
1:A:202:GLN:O	1:A:203:ARG:CG	0.42	2.67	15	1
1:A:201:LYS:CE	1:A:219:ARG:C	0.42	2.92	6	1
1:A:130:PHE:CZ	1:A:150:LEU:CD2	0.42	2.99	7	1
1:A:79:LEU:CD1	1:A:80:ILE:CD1	0.42	2.97	11	1
1:A:228:LEU:O	1:A:228:LEU:HD23	0.42	2.14	14	1
1:A:229:CYS:SG	1:A:236:MET:HG3	0.42	2.53	1	1
1:A:160:ASN:OD1	1:A:160:ASN:C	0.42	2.62	3	1
1:A:226:ALA:O	1:A:227:PHE:CD1	0.42	2.73	3	1
1:A:164:ASP:HB3	1:A:205:ILE:CG1	0.42	2.44	7	1
1:A:191:HIS:CG	1:A:228:LEU:CD2	0.42	3.02	7	1
1:A:192:LEU:HD13	1:A:229:CYS:O	0.42	2.14	8	1
1:A:203:ARG:NE	1:A:218:ASP:HB2	0.42	2.29	8	1
1:A:130:PHE:CD1	1:A:150:LEU:HD11	0.42	2.49	10	1
1:A:91:THR:O	1:A:91:THR:CG2	0.42	2.66	15	1
1:A:168:ILE:O	1:A:200:THR:CB	0.42	2.67	15	1
1:A:157:LEU:CD2	1:A:158:PRO:HD2	0.42	2.44	9	1
1:A:167:LEU:CD1	1:A:202:GLN:HB3	0.42	2.43	13	1
1:A:161:ALA:CB	1:A:206:LYS:HE2	0.42	2.45	1	1
1:A:96:SER:O	1:A:99:VAL:HG12	0.42	2.15	5	1
1:A:141:LEU:N	1:A:141:LEU:CD2	0.42	2.83	8	1
1:A:190:GLU:O	1:A:230:ASP:OD1	0.42	2.37	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:202:GLN:O	1:A:202:GLN:HG3	0.42	2.15	9	1
1:A:118:LYS:O	1:A:121:GLU:HB2	0.42	2.14	11	1
1:A:120:ILE:HA	1:A:123:TYR:CB	0.42	2.45	13	1
1:A:204:LEU:O	1:A:204:LEU:CG	0.42	2.67	15	1
1:A:136:SER:O	1:A:139:LYS:CB	0.42	2.68	2	1
1:A:85:LEU:O	1:A:89:LEU:HB2	0.42	2.15	3	2
1:A:149:ALA:O	1:A:150:LEU:C	0.42	2.60	13	2
1:A:142:VAL:CG1	1:A:147:GLN:N	0.42	2.82	8	1
1:A:176:LEU:HD22	1:A:196:TYR:CG	0.42	2.50	9	1
1:A:192:LEU:HD12	1:A:192:LEU:N	0.42	2.27	10	1
1:A:199:ASP:OD2	1:A:222:VAL:CG1	0.42	2.60	12	1
1:A:129:SER:OG	1:A:134:ASN:HB3	0.42	2.15	15	1
1:A:199:ASP:C	1:A:200:THR:CG2	0.42	2.93	2	1
1:A:203:ARG:HG3	1:A:218:ASP:CA	0.42	2.45	13	2
1:A:223:ASP:HB3	1:A:225:ILE:HD11	0.42	1.92	6	1
1:A:91:THR:OG1	1:A:95:ASN:HB2	0.42	2.15	12	2
1:A:228:LEU:O	1:A:237:ILE:HB	0.42	2.15	11	2
1:A:242:LEU:C	1:A:242:LEU:CD1	0.42	2.81	11	1
1:A:202:GLN:NE2	1:A:204:LEU:CD2	0.42	2.83	15	1
1:A:202:GLN:O	1:A:203:ARG:HG2	0.42	2.14	15	1
1:A:101:LEU:C	1:A:103:ARG:N	0.42	2.77	4	1
1:A:129:SER:HA	1:A:133:LYS:O	0.42	2.14	7	1
1:A:176:LEU:CD2	1:A:196:TYR:CD2	0.42	3.03	9	1
1:A:175:LYS:HA	1:A:176:LEU:CD1	0.42	2.39	12	1
1:A:176:LEU:CD2	1:A:197:LYS:CB	0.42	2.93	15	1
1:A:92:PHE:HB3	1:A:95:ASN:HB3	0.42	1.91	9	2
1:A:129:SER:O	1:A:134:ASN:N	0.42	2.53	9	1
1:A:153:ARG:CG	1:A:154:SER:N	0.42	2.82	12	1
1:A:133:LYS:O	1:A:134:ASN:CB	0.42	2.68	13	1
1:A:229:CYS:HB3	1:A:236:MET:HA	0.42	1.92	14	1
1:A:158:PRO:HD2	1:A:161:ALA:CB	0.42	2.44	15	1
1:A:229:CYS:SG	1:A:236:MET:HG2	0.41	2.55	1	1
1:A:131:ALA:CB	1:A:165:TRP:N	0.41	2.83	8	1
1:A:152:ALA:O	1:A:155:ARG:HG3	0.41	2.15	8	1
1:A:138:ILE:HG22	1:A:142:VAL:CG2	0.41	2.44	13	1
1:A:144:LEU:C	1:A:144:LEU:CD2	0.41	2.75	13	1
1:A:122:THR:C	1:A:124:ILE:N	0.41	2.78	14	1
1:A:124:ILE:HG13	1:A:167:LEU:CD2	0.41	2.45	14	1
1:A:170:PHE:O	1:A:171:ASN:HB3	0.41	2.15	14	1
1:A:89:LEU:HD13	1:A:89:LEU:O	0.41	2.15	15	1
1:A:194:LEU:HD12	1:A:196:TYR:OH	0.41	2.15	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:220:ASP:O	1:A:220:ASP:CG	0.41	2.63	14	3
1:A:207:VAL:O	1:A:207:VAL:CG2	0.41	2.66	5	1
1:A:95:ASN:ND2	1:A:99:VAL:HG23	0.41	2.30	6	1
1:A:156:GLN:O	1:A:157:LEU:HG	0.41	2.14	7	2
1:A:143:SER:HB3	1:A:146:VAL:CG1	0.41	2.44	9	1
1:A:190:GLU:HB3	1:A:230:ASP:CB	0.41	2.45	9	1
1:A:128:THR:HG22	1:A:133:LYS:CD	0.41	2.44	10	1
1:A:98:GLN:O	1:A:101:LEU:CD2	0.41	2.69	4	1
1:A:162:THR:O	1:A:206:LYS:HG3	0.41	2.15	5	1
1:A:127:ASN:C	1:A:165:TRP:HB3	0.41	2.40	6	1
1:A:228:LEU:HB3	1:A:237:ILE:HG12	0.41	1.92	12	1
1:A:192:LEU:CD2	1:A:229:CYS:HB3	0.41	2.44	4	1
1:A:197:LYS:CG	1:A:224:TYR:CE2	0.41	3.04	7	1
1:A:81:VAL:O	1:A:85:LEU:HB2	0.41	2.15	10	1
1:A:135:LEU:C	1:A:138:ILE:HG22	0.41	2.40	15	1
1:A:168:ILE:HB	1:A:201:LYS:CB	0.41	2.45	1	1
1:A:83:ASN:O	1:A:87:ARG:HB2	0.41	2.15	2	1
1:A:129:SER:O	1:A:130:PHE:C	0.41	2.61	2	1
1:A:136:SER:O	1:A:139:LYS:HB3	0.41	2.16	15	2
1:A:163:LEU:HA	1:A:205:ILE:O	0.41	2.14	2	1
1:A:225:ILE:HA	1:A:240:GLY:HA3	0.41	1.91	5	1
1:A:173:VAL:CG2	1:A:197:LYS:HD3	0.41	2.45	7	1
1:A:138:ILE:HG21	1:A:147:GLN:HG3	0.41	1.91	14	1
1:A:168:ILE:HG13	1:A:201:LYS:O	0.41	2.16	1	3
1:A:192:LEU:HB2	1:A:229:CYS:SG	0.41	2.55	7	1
1:A:123:TYR:CD1	1:A:198:PHE:CE2	0.41	3.08	13	1
1:A:192:LEU:HD23	1:A:194:LEU:HD23	0.41	1.92	14	1
1:A:192:LEU:HB3	1:A:194:LEU:CD1	0.41	2.46	15	1
1:A:88:ARG:HA	1:A:91:THR:OG1	0.41	2.15	2	1
1:A:101:LEU:O	1:A:103:ARG:N	0.41	2.54	4	1
1:A:176:LEU:O	1:A:176:LEU:CD2	0.41	2.64	5	1
1:A:167:LEU:O	1:A:167:LEU:CD2	0.41	2.58	15	1
1:A:228:LEU:CD2	1:A:237:ILE:CG1	0.41	2.97	15	1
1:A:150:LEU:O	1:A:151:GLU:C	0.41	2.64	1	1
1:A:91:THR:O	1:A:92:PHE:C	0.41	2.60	5	1
1:A:165:TRP:CD1	1:A:165:TRP:N	0.41	2.88	9	1
1:A:174:PRO:HB3	1:A:198:PHE:HA	0.41	1.93	9	1
1:A:158:PRO:HG3	1:A:161:ALA:CB	0.41	2.44	10	1
1:A:168:ILE:CD1	1:A:202:GLN:CD	0.41	2.94	15	1
1:A:164:ASP:HB3	1:A:205:ILE:CG2	0.41	2.46	1	1
1:A:144:LEU:O	1:A:148:GLU:CB	0.41	2.68	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:208:ASN:OD1	1:A:213:LYS:HB3	0.41	2.16	2	1
1:A:197:LYS:HD2	1:A:224:TYR:CE2	0.41	2.51	3	1
1:A:206:LYS:HG2	1:A:207:VAL:N	0.41	2.31	3	1
1:A:167:LEU:HD12	1:A:202:GLN:HB3	0.41	1.91	5	1
1:A:167:LEU:HD23	1:A:200:THR:HB	0.41	1.93	7	1
1:A:141:LEU:N	1:A:141:LEU:HD22	0.41	2.29	8	1
1:A:169:LYS:HA	1:A:200:THR:CG2	0.41	2.46	8	1
1:A:132:HIS:O	1:A:133:LYS:HB3	0.41	2.16	9	1
1:A:86:ILE:HA	1:A:89:LEU:HB3	0.41	1.92	10	1
1:A:81:VAL:O	1:A:82:ALA:C	0.41	2.64	11	1
1:A:204:LEU:O	1:A:205:ILE:HG13	0.41	2.15	15	1
1:A:165:TRP:O	1:A:167:LEU:CD1	0.41	2.65	1	1
1:A:230:ASP:O	1:A:235:ASP:CB	0.41	2.69	1	1
1:A:92:PHE:CD2	1:A:95:ASN:HB3	0.41	2.51	2	1
1:A:99:VAL:O	1:A:102:PHE:CE1	0.41	2.74	2	1
1:A:162:THR:HB	1:A:207:VAL:CG2	0.41	2.46	2	1
1:A:79:LEU:HD12	1:A:80:ILE:CD1	0.41	2.46	11	1
1:A:88:ARG:HD2	1:A:92:PHE:CE2	0.41	2.50	11	1
1:A:197:LYS:C	1:A:197:LYS:CD	0.41	2.94	11	1
1:A:165:TRP:CZ3	1:A:202:GLN:OE1	0.41	2.74	14	1
1:A:98:GLN:O	1:A:101:LEU:HB2	0.40	2.15	2	2
1:A:133:LYS:O	1:A:133:LYS:CG	0.40	2.68	5	1
1:A:91:THR:HG22	1:A:95:ASN:OD1	0.40	2.16	6	1
1:A:173:VAL:HB	1:A:199:ASP:CB	0.40	2.46	7	1
1:A:146:VAL:HG21	1:A:238:LEU:O	0.40	2.16	10	1
1:A:128:THR:HA	1:A:165:TRP:CE3	0.40	2.51	11	1
1:A:192:LEU:O	1:A:228:LEU:HG	0.40	2.16	12	1
1:A:243:PHE:CD1	1:A:243:PHE:N	0.40	2.88	13	1
1:A:81:VAL:CG1	1:A:82:ALA:N	0.40	2.84	14	1
1:A:166:GLN:O	1:A:166:GLN:CG	0.40	2.68	15	1
1:A:130:PHE:C	1:A:132:HIS:N	0.40	2.79	2	1
1:A:165:TRP:CE3	1:A:165:TRP:HA	0.40	2.52	4	1
1:A:136:SER:O	1:A:138:ILE:N	0.40	2.54	6	1
1:A:203:ARG:CZ	1:A:216:THR:HG22	0.40	2.46	7	1
1:A:147:GLN:CD	1:A:151:GLU:CD	0.40	2.89	9	1
1:A:175:LYS:C	1:A:176:LEU:CG	0.40	2.94	13	1
1:A:124:ILE:HA	1:A:167:LEU:CD2	0.40	2.43	14	1
1:A:165:TRP:O	1:A:166:GLN:C	0.40	2.64	2	1
1:A:203:ARG:NH2	1:A:216:THR:HB	0.40	2.31	2	1
1:A:198:PHE:CD1	1:A:225:ILE:CG1	0.40	3.03	5	1
1:A:136:SER:C	1:A:138:ILE:N	0.40	2.78	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:204:LEU:HD23	1:A:204:LEU:C	0.40	2.42	8	1
1:A:142:VAL:O	1:A:143:SER:HB2	0.40	2.15	9	1
1:A:202:GLN:O	1:A:218:ASP:HA	0.40	2.16	9	1
1:A:83:ASN:OD1	1:A:83:ASN:C	0.40	2.63	10	1
1:A:163:LEU:O	1:A:163:LEU:HD13	0.40	2.16	2	1
1:A:146:VAL:CG2	1:A:239:MET:HA	0.40	2.46	8	1
1:A:242:LEU:CD1	1:A:242:LEU:H	0.40	2.29	2	1
1:A:116:LYS:HG2	1:A:117:ASN:N	0.40	2.30	3	1
1:A:98:GLN:O	1:A:99:VAL:C	0.40	2.65	4	1
1:A:130:PHE:CZ	1:A:150:LEU:HG	0.40	2.52	4	1
1:A:227:PHE:CD1	1:A:228:LEU:N	0.40	2.89	6	1
1:A:227:PHE:CE1	1:A:229:CYS:CB	0.40	3.05	6	1
1:A:123:TYR:CD2	1:A:198:PHE:CD2	0.40	3.09	14	1
1:A:201:LYS:HD3	1:A:219:ARG:C	0.40	2.42	14	1
1:A:207:VAL:HA	1:A:213:LYS:O	0.40	2.17	14	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	135/210 (64%)	115±2 (85±2%)	13±3 (10±2%)	7±2 (5±1%)	3	23
All	All	2025/3150 (64%)	1722 (85%)	197 (10%)	106 (5%)	3	23

All 22 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	156	GLN	13
1	A	157	LEU	13
1	A	172	ALA	11
1	A	158	PRO	10
1	A	142	VAL	9
1	A	133	LYS	6
1	A	171	ASN	6

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Mol	Chain	Res	Type	Models (Total)
1	A	91	THR	5
1	A	92	PHE	4
1	A	231	ALA	4
1	A	134	ASN	4
1	A	190	GLU	3
1	A	243	PHE	3
1	A	213	LYS	3
1	A	160	ASN	3
1	A	78	PRO	2
1	A	235	ASP	2
1	A	143	SER	1
1	A	132	HIS	1
1	A	159	GLY	1
1	A	166	GLN	1
1	A	165	TRP	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/189 (63%)	97±4 (81±3%)	23±4 (19±3%)	3	34
All	All	1800/2835 (63%)	1456 (81%)	344 (19%)	3	34

All 90 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	167	LEU	13
1	A	157	LEU	11
1	A	204	LEU	11
1	A	242	LEU	11
1	A	79	LEU	11
1	A	217	LEU	11
1	A	228	LEU	11
1	A	239	MET	10
1	A	176	LEU	9
1	A	197	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	200	THR	9
1	A	192	LEU	9
1	A	238	LEU	8
1	A	194	LEU	7
1	A	92	PHE	6
1	A	101	LEU	6
1	A	235	ASP	6
1	A	236	MET	6
1	A	163	LEU	6
1	A	193	GLN	6
1	A	116	LYS	5
1	A	145	TRP	5
1	A	150	LEU	5
1	A	144	LEU	5
1	A	223	ASP	5
1	A	88	ARG	5
1	A	132	HIS	5
1	A	133	LYS	5
1	A	91	THR	4
1	A	137	ASP	4
1	A	191	HIS	4
1	A	213	LYS	4
1	A	89	LEU	4
1	A	118	LYS	4
1	A	143	SER	4
1	A	162	THR	4
1	A	120	ILE	4
1	A	201	LYS	4
1	A	134	ASN	4
1	A	129	SER	3
1	A	229	CYS	3
1	A	225	ILE	3
1	A	227	PHE	3
1	A	139	LYS	3
1	A	142	VAL	3
1	A	85	LEU	2
1	A	138	ILE	2
1	A	243	PHE	2
1	A	80	ILE	2
1	A	122	THR	2
1	A	164	ASP	2
1	A	170	PHE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	90	TYR	2
1	A	141	LEU	2
1	A	171	ASN	2
1	A	94	LEU	2
1	A	86	ILE	2
1	A	96	SER	2
1	A	199	ASP	2
1	A	190	GLU	2
1	A	205	ILE	2
1	A	98	GLN	2
1	A	166	GLN	2
1	A	135	LEU	2
1	A	237	ILE	2
1	A	87	ARG	2
1	A	202	GLN	1
1	A	125	ASN	1
1	A	156	GLN	1
1	A	95	ASN	1
1	A	169	LYS	1
1	A	206	LYS	1
1	A	130	PHE	1
1	A	155	ARG	1
1	A	160	ASN	1
1	A	168	ILE	1
1	A	203	ARG	1
1	A	241	SER	1
1	A	123	TYR	1
1	A	153	ARG	1
1	A	154	SER	1
1	A	177	VAL	1
1	A	127	ASN	1
1	A	215	GLU	1
1	A	148	GLU	1
1	A	175	LYS	1
1	A	124	ILE	1
1	A	103	ARG	1
1	A	121	GLU	1
1	A	151	GLU	1

6.3.3 RNA ⓘ

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 51% for the well-defined parts and 49% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	1586
Number of shifts mapped to atoms	1469
Number of unparsed shifts	0
Number of shifts with mapping errors	117
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 117 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	35	LYS	H	8.249	0.001	1
1	A	35	LYS	HA	4.297	.	1
1	A	35	LYS	HB2	1.895	.	1
1	A	35	LYS	HD2	1.74	.	1
1	A	35	LYS	HG2	1.404	.	1
1	A	35	LYS	C	175.731	.	1
1	A	35	LYS	CA	55.542	.	1
1	A	35	LYS	CB	31.445	.	1
1	A	35	LYS	N	123.012	0.065	1
1	A	36	GLU	H	7.998	0.002	1
1	A	36	GLU	HA	4.021	.	1
1	A	36	GLU	HB2	1.972	.	1
1	A	36	GLU	HG2	2.248	.	1
1	A	36	GLU	C	178.519	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	36	GLU	CA	56.261	.	1
1	A	36	GLU	CB	28.282	.	1
1	A	36	GLU	N	119.073	0.067	1
1	A	37	SER	H	8.257	0.004	1
1	A	37	SER	HA	4.452	.	1
1	A	37	SER	HB2	3.866	.	1
1	A	37	SER	C	174.298	.	1
1	A	37	SER	CA	57.76	.	1
1	A	37	SER	CB	62.721	.	1
1	A	37	SER	N	116.674	0.057	1
1	A	39	THR	H	8.133	0.005	1
1	A	39	THR	HA	4.367	.	1
1	A	39	THR	HB	4.021	.	1
1	A	39	THR	HG21	1.15	0.004	1
1	A	39	THR	HG22	1.15	0.004	1
1	A	39	THR	HG23	1.15	0.004	1
1	A	39	THR	C	174.573	.	1
1	A	39	THR	CA	61.627	0.0	1
1	A	39	THR	CB	68.559	0.018	1
1	A	39	THR	CG2	19.385	.	1
1	A	39	THR	N	114.601	0.056	1
1	A	44	ASP	H	8.25	0.002	1
1	A	44	ASP	HA	4.297	.	1
1	A	44	ASP	HB2	2.558	.	1
1	A	44	ASP	C	175.855	.	1
1	A	44	ASP	CA	53.373	.	1
1	A	44	ASP	CB	40.321	.	1
1	A	44	ASP	N	122.094	0.01	1
1	A	48	GLN	H	8.183	0.002	1
1	A	48	GLN	HA	3.93	.	1
1	A	48	GLN	HB2	2.015	.	1
1	A	48	GLN	C	174.959	.	1
1	A	48	GLN	CA	54.96	0.062	1
1	A	48	GLN	CB	27.981	0.028	1
1	A	48	GLN	N	120.807	0.029	1
1	A	51	PHE	H	8.207	0.004	1
1	A	51	PHE	HA	4.331	.	1
1	A	51	PHE	HB2	3.049	.	1
1	A	51	PHE	C	173.911	.	1
1	A	51	PHE	CA	56.527	0.011	1
1	A	51	PHE	CB	38.253	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	PHE	N	120.857	0.054	1
1	A	52	ASN	H	8.216	0.001	1
1	A	52	ASN	HA	4.443	.	1
1	A	52	ASN	HB2	2.678	.	1
1	A	52	ASN	C	173.057	.	1
1	A	52	ASN	CA	49.954	.	1
1	A	52	ASN	CB	38.1	.	1
1	A	52	ASN	N	122.645	0.048	1
1	A	55	HIS	H	7.599	0.004	1
1	A	55	HIS	HA	4.409	.	1
1	A	55	HIS	HB2	3.238	.	1
1	A	55	HIS	C	175.193	.	1
1	A	55	HIS	CA	56.599	.	1
1	A	55	HIS	CB	28.465	.	1
1	A	55	HIS	N	119.437	0.072	1
1	A	57	GLY	H	8.215	0.011	1
1	A	57	GLY	HA2	3.996	.	2
1	A	57	GLY	HA3	3.915	.	2
1	A	57	GLY	C	174.146	.	1
1	A	57	GLY	CA	44.845	0.001	1
1	A	57	GLY	N	108.255	0.101	1
1	A	58	VAL	H	7.91	0.004	1
1	A	58	VAL	HA	3.944	.	1
1	A	58	VAL	HB	2.127	.	1
1	A	58	VAL	HG11	0.945	0.012	1
1	A	58	VAL	HG12	0.945	0.012	1
1	A	58	VAL	HG13	0.945	0.012	1
1	A	58	VAL	C	175.646	.	1
1	A	58	VAL	CA	61.967	.	1
1	A	58	VAL	CB	31.009	.	1
1	A	58	VAL	CG1	18.386	.	1
1	A	58	VAL	N	119.622	0.012	1
1	A	59	ALA	H	7.897	0.004	1
1	A	59	ALA	HA	4.297	.	1
1	A	59	ALA	HB1	1.348	0.005	1
1	A	59	ALA	HB2	1.348	0.005	1
1	A	59	ALA	HB3	1.348	0.005	1
1	A	59	ALA	C	177.126	.	1
1	A	59	ALA	CA	52.288	.	1
1	A	59	ALA	CB	17.446	.	1
1	A	59	ALA	N	123.04	0.106	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	62	ILE	H	7.628	0.009	1
1	A	62	ILE	HA	4.169	.	1
1	A	62	ILE	HB	1.762	.	1
1	A	62	ILE	HD11	0.659	.	1
1	A	62	ILE	HD12	0.659	.	1
1	A	62	ILE	HD13	0.659	.	1
1	A	62	ILE	HG21	0.865	0.001	1
1	A	62	ILE	HG22	0.865	0.001	1
1	A	62	ILE	HG23	0.865	0.001	1
1	A	62	ILE	C	174.94	.	1
1	A	62	ILE	CA	60.948	0.015	1
1	A	62	ILE	CB	37.072	0.003	1
1	A	62	ILE	CG2	15.186	.	1
1	A	62	ILE	N	117.534	0.082	1
1	A	64	ILE	HG12	1.14	.	1
1	A	68	TYR	H	7.795	0.002	1
1	A	68	TYR	HA	4.224	.	1
1	A	68	TYR	HB2	2.914	.	1
1	A	68	TYR	CA	57.35	0.016	1
1	A	68	TYR	CB	37.045	0.002	1
1	A	68	TYR	N	116.155	0.039	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	162	0.59 ± 0.16	Should be checked
$^{13}\text{C}_\beta$	153	1.54 ± 0.09	Should be checked
$^{13}\text{C}'$	140	0.56 ± 0.10	Should be applied
^{15}N	189	0.19 ± 0.16	None needed (< 0.5 ppm)

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 51%, i.e. 991 atoms were assigned a chemical shift out of a possible 1959. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	507/673 (75%)	224/271 (83%)	171/270 (63%)	112/132 (85%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	484/1142 (42%)	329/747 (44%)	155/349 (44%)	0/46 (0%)
Aromatic	0/144 (0%)	0/71 (0%)	0/69 (0%)	0/4 (0%)
Overall	991/1959 (51%)	553/1089 (51%)	326/688 (47%)	112/182 (62%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 49%, i.e. 1468 atoms were assigned a chemical shift out of a possible 3004. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	798/1033 (77%)	348/415 (84%)	275/420 (65%)	175/198 (88%)
Sidechain	670/1753 (38%)	446/1144 (39%)	224/540 (41%)	0/69 (0%)
Aromatic	0/218 (0%)	0/108 (0%)	0/103 (0%)	0/7 (0%)
Overall	1468/3004 (49%)	794/1667 (48%)	499/1063 (47%)	175/274 (64%)

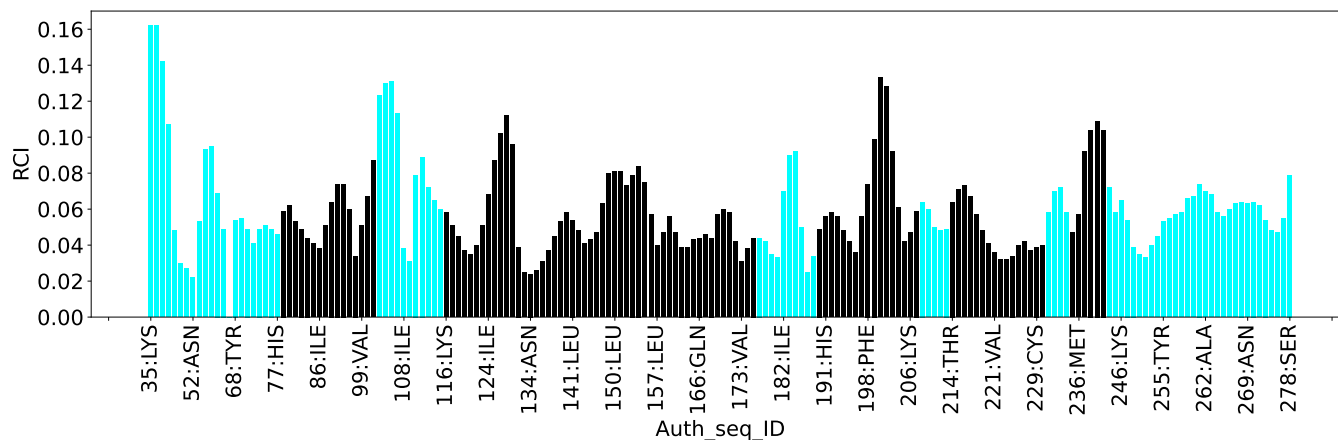
7.1.4 Statistically unusual chemical shifts [i](#)

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	399
Intra-residue ($ i-j =0$)	1
Sequential ($ i-j =1$)	216
Medium range ($ i-j >1$ and $ i-j <5$)	63
Long range ($ i-j \geq 5$)	119
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	264
Number of unmapped restraints	0
Number of restraints per residue	3.2
Number of long range restraints per residue ¹	0.6

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	1.6	0.2
0.2-0.5 (Medium)	6.1	0.5
>0.5 (Large)	88.3	48.03

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)	16.4	9.96
10.0-20.0 (Medium)	3.5	19.75
>20.0 (Large)	39.6	159.91

9 Distance violation analysis ⓘ

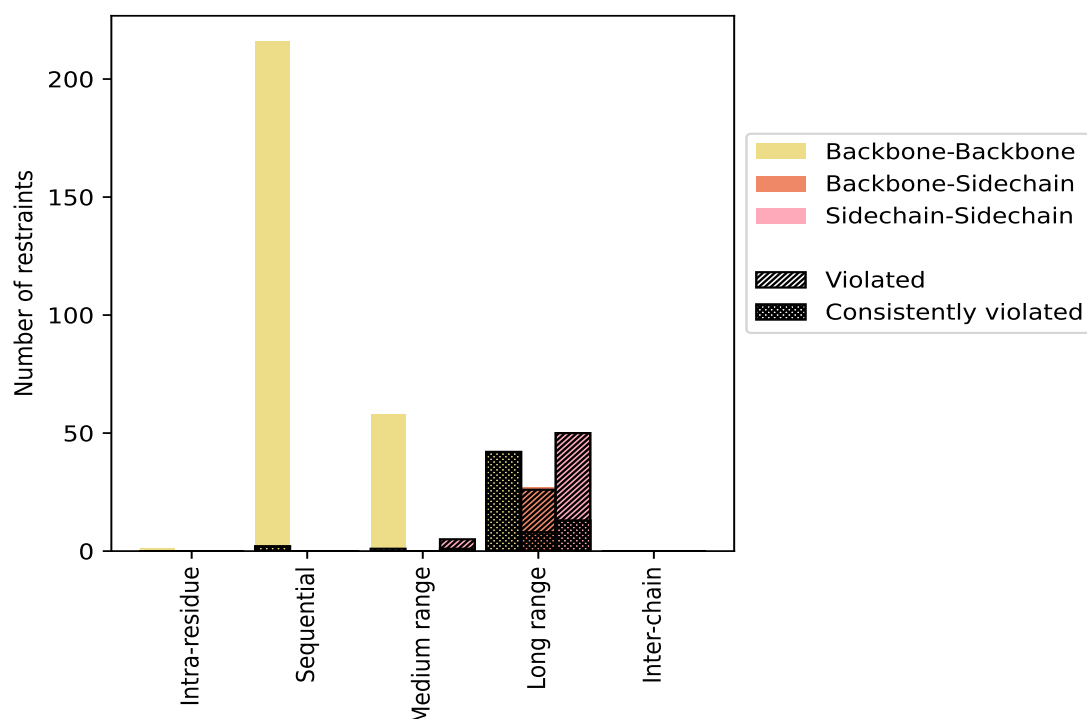
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	1	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	216	54.1	2	0.9	0.5	2	0.9	0.5
Backbone-Backbone	216	54.1	2	0.9	0.5	2	0.9	0.5
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	63	15.8	6	9.5	1.5	1	1.6	0.3
Backbone-Backbone	58	14.5	1	1.7	0.3	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	5	1.3	5	100.0	1.3	1	20.0	0.3
Long range ($i-j \geq 5$)	119	29.8	118	99.2	29.6	63	52.9	15.8
Backbone-Backbone	42	10.5	42	100.0	10.5	42	100.0	10.5
Backbone-Sidechain	27	6.8	26	96.3	6.5	8	29.6	2.0
Sidechain-Sidechain	50	12.5	50	100.0	12.5	13	26.0	3.3
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	399	100.0	126	31.6	31.6	66	16.5	16.5
Backbone-Backbone	317	79.4	45	14.2	11.3	44	13.9	11.0
Backbone-Sidechain	27	6.8	26	96.3	6.5	8	29.6	2.0
Sidechain-Sidechain	55	13.8	55	100.0	13.8	14	25.5	3.5

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	2	2	85	0	89	12.51	41.97	10.38	13.9
2	0	2	2	91	0	95	10.99	31.34	9.46	12.31
3	0	2	3	92	0	97	11.58	33.48	9.96	12.61
4	0	2	4	93	0	99	10.98	34.78	9.66	10.13
5	0	2	4	90	0	96	11.2	39.92	10.03	9.04
6	0	2	4	94	0	100	10.6	30.01	9.11	8.92
7	0	2	2	89	0	93	11.96	40.79	10.3	13.46
8	0	2	4	93	0	99	11.04	36.57	10.06	9.56
9	0	2	4	91	0	97	11.17	37.7	10.06	11.77
10	0	2	3	90	0	95	11.47	38.88	9.85	11.68

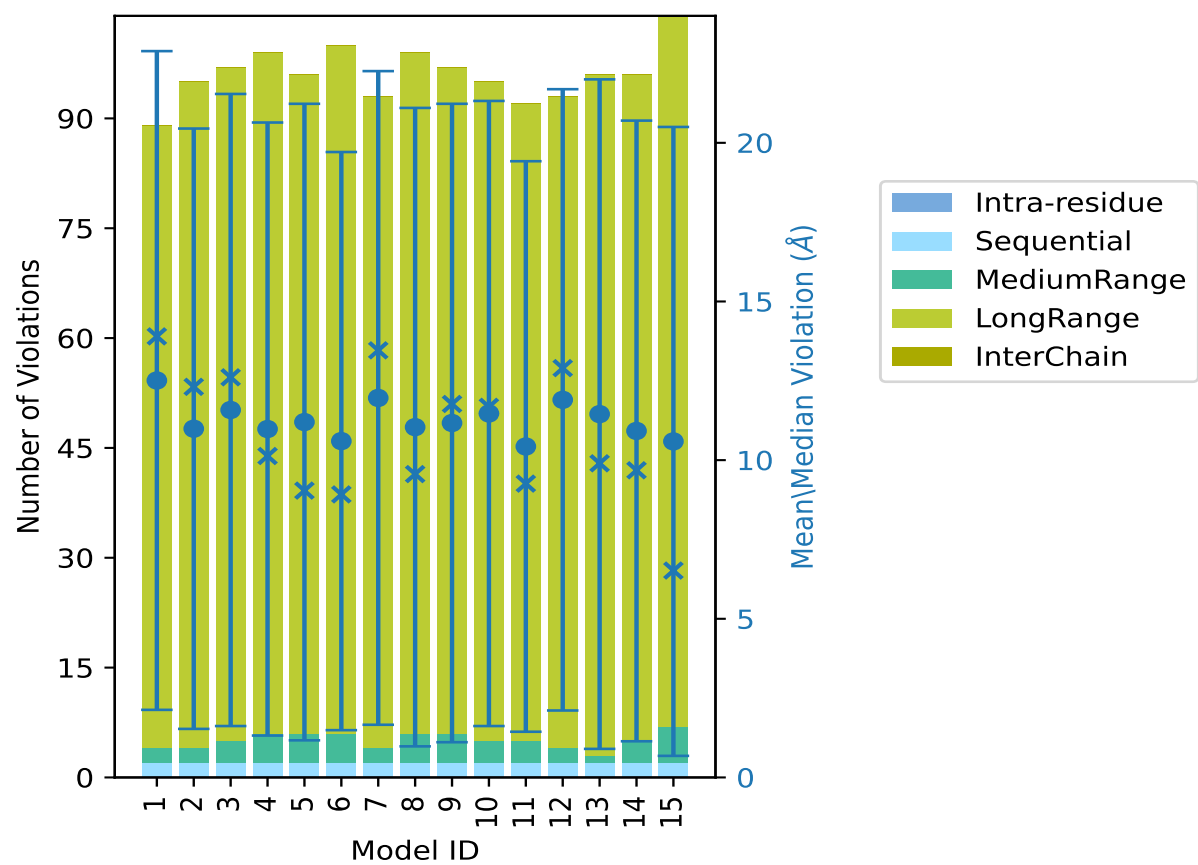
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	2	3	87	0	92	10.43	31.04	8.99	9.26
12	0	2	2	89	0	93	11.9	36.06	9.79	12.9
13	0	2	1	93	0	96	11.45	48.03	10.55	9.9
14	0	2	3	91	0	96	10.92	37.4	9.78	9.68
15	0	2	5	97	0	104	10.59	33.89	9.91	6.52

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

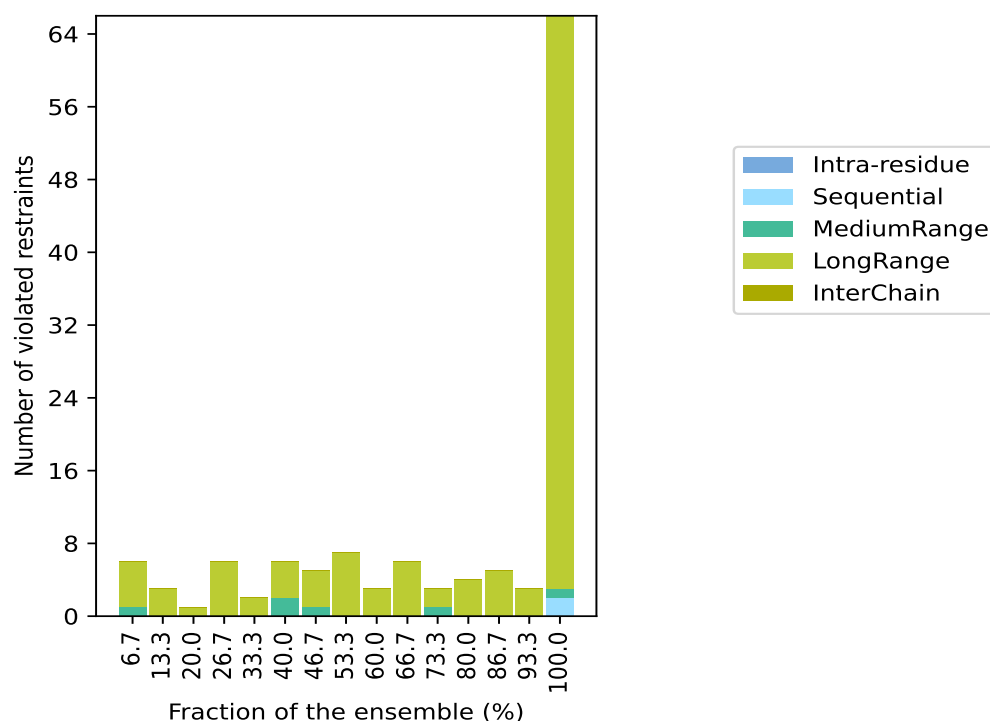
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 273(IR:1, SQ:214, MR:57, LR:1, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	1	5	0	6	1	6.7
0	0	0	3	0	3	2	13.3
0	0	0	1	0	1	3	20.0
0	0	0	6	0	6	4	26.7
0	0	0	2	0	2	5	33.3
0	0	2	4	0	6	6	40.0
0	0	1	4	0	5	7	46.7
0	0	0	7	0	7	8	53.3
0	0	0	3	0	3	9	60.0
0	0	0	6	0	6	10	66.7
0	0	1	2	0	3	11	73.3
0	0	0	4	0	4	12	80.0
0	0	0	5	0	5	13	86.7
0	0	0	3	0	3	14	93.3
0	2	1	63	0	66	15	100.0

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

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

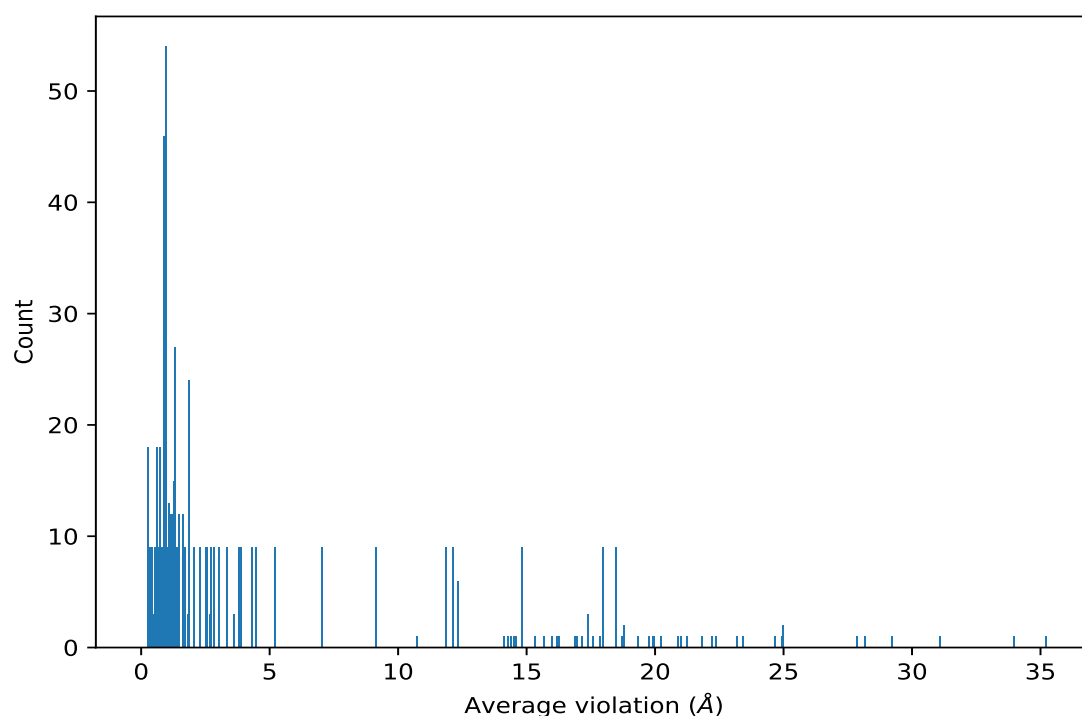
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	15	35.22	7.48	36.57
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	15	33.96	6.95	35.89
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	15	31.09	0.53	31.04
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	15	29.21	0.41	29.16
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	15	28.16	0.45	28.25
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	15	27.88	0.59	27.85
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	15	24.98	0.33	24.97
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	15	24.97	2.92	24.38
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	15	24.93	0.41	24.83
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	15	24.65	3.18	23.65
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	15	23.43	1.74	23.25
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	15	23.18	1.68	22.77
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	15	22.39	0.79	22.19
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	15	22.21	0.81	22.1
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	15	21.84	0.98	21.8
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	15	21.21	0.95	21.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	15	21.0	2.46	20.74
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	15	20.86	0.7	20.62
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	15	20.2	1.04	20.16
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	15	19.98	0.95	19.88
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	15	19.93	0.89	19.79
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	15	19.75	2.12	18.96
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	15	19.32	1.17	18.98
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	15	18.75	0.71	18.69
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	15	18.75	0.57	18.75
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	15	18.72	1.93	17.97
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	15	18.46	6.49	20.06
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	15	18.46	6.49	20.06
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	15	18.46	6.49	20.06
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	15	18.46	6.49	20.06
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	15	18.46	6.49	20.06
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	15	18.46	6.49	20.06
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	15	18.46	6.49	20.06
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	15	18.46	6.49	20.06
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	15	18.46	6.49	20.06
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	15	17.97	6.31	18.19
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	15	17.97	6.31	18.19
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	15	17.97	6.31	18.19
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	15	17.97	6.31	18.19
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	15	17.97	6.31	18.19
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	15	17.97	6.31	18.19
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	15	17.97	6.31	18.19
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	15	17.97	6.31	18.19
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	15	17.97	6.31	18.19
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	15	17.89	1.1	18.12
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	15	17.59	0.34	17.51
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	15	17.37	1.97	18.05
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	15	17.37	1.97	18.05
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	15	17.37	1.97	18.05
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	15	17.18	0.77	16.85
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	15	16.96	0.79	16.88
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	15	16.86	0.94	16.8
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	15	16.25	1.23	16.25
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	15	16.17	1.36	16.72
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	15	15.95	2.35	15.57
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	15	15.65	0.7	15.81
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	15	15.31	1.7	14.95
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	15	14.8	0.8	14.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	15	14.8	0.8	14.86
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	15	14.8	0.8	14.86
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	15	14.8	0.8	14.86
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	15	14.8	0.8	14.86
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	15	14.8	0.8	14.86
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	15	14.8	0.8	14.86
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	15	14.8	0.8	14.86
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	15	14.8	0.8	14.86
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	15	14.57	1.51	14.93
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	15	14.54	1.44	14.05
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	15	14.35	0.98	14.48
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	15	14.29	1.81	14.56
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	15	14.1	1.15	14.13
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	15	12.32	2.11	12.71
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	15	12.32	2.11	12.71
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	15	12.32	2.11	12.71
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	15	12.32	2.11	12.71
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	15	12.32	2.11	12.71
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	15	12.32	2.11	12.71
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	15	12.11	1.35	12.27
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	15	12.11	1.35	12.27
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	15	12.11	1.35	12.27
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	15	12.11	1.35	12.27
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	15	12.11	1.35	12.27
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	15	12.11	1.35	12.27
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	15	12.11	1.35	12.27
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	15	12.11	1.35	12.27
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	15	12.11	1.35	12.27
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	15	11.86	2.36	12.16
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	15	11.86	2.36	12.16
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	15	11.86	2.36	12.16
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	15	11.86	2.36	12.16
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	15	11.86	2.36	12.16
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	15	11.86	2.36	12.16
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	15	11.86	2.36	12.16
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	15	11.86	2.36	12.16
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	15	11.86	2.36	12.16
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	15	10.71	1.18	10.38
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	15	9.12	2.54	9.45
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	15	9.12	2.54	9.45
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	15	9.12	2.54	9.45
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	15	9.12	2.54	9.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	15	9.12	2.54	9.45
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	15	9.12	2.54	9.45
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	15	9.12	2.54	9.45
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	15	9.12	2.54	9.45
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	15	9.12	2.54	9.45
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	15	7.03	1.39	7.1
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	15	7.03	1.39	7.1
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	15	7.03	1.39	7.1
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	15	7.03	1.39	7.1
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	15	7.03	1.39	7.1
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	15	7.03	1.39	7.1
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	15	7.03	1.39	7.1
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	15	7.03	1.39	7.1
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	15	7.03	1.39	7.1
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	15	5.21	1.09	5.08
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	15	5.21	1.09	5.08
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	15	5.21	1.09	5.08
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	15	5.21	1.09	5.08
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	15	5.21	1.09	5.08
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	15	5.21	1.09	5.08
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	15	5.21	1.09	5.08
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	15	5.21	1.09	5.08
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	15	5.21	1.09	5.08
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	15	4.33	1.51	4.69
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	15	4.33	1.51	4.69
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	15	4.33	1.51	4.69
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	15	4.33	1.51	4.69
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	15	4.33	1.51	4.69
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	15	4.33	1.51	4.69
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	15	4.33	1.51	4.69
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	15	4.33	1.51	4.69
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	15	4.33	1.51	4.69
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	15	3.86	1.27	3.7
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	15	3.86	1.27	3.7
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	15	3.86	1.27	3.7
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	15	3.86	1.27	3.7
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	15	3.86	1.27	3.7
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	15	3.86	1.27	3.7
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	15	3.86	1.27	3.7
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	15	3.86	1.27	3.7
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	15	3.86	1.27	3.7
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	15	3.82	1.45	3.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	15	3.82	1.45	3.57
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	15	3.82	1.45	3.57
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	15	3.82	1.45	3.57
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	15	3.82	1.45	3.57
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	15	3.82	1.45	3.57
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	15	3.82	1.45	3.57
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	15	3.82	1.45	3.57
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	15	3.82	1.45	3.57
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	15	3.61	1.26	3.33
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	15	3.61	1.26	3.33
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	15	3.61	1.26	3.33
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	15	2.66	1.03	2.97
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	15	2.66	1.03	2.97
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	15	2.66	1.03	2.97
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	15	2.26	1.41	2.06
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	15	2.26	1.41	2.06
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	15	2.26	1.41	2.06
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	15	2.26	1.41	2.06
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	15	2.26	1.41	2.06
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	15	2.26	1.41	2.06
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	15	2.26	1.41	2.06
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	15	2.26	1.41	2.06
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	15	2.26	1.41	2.06
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	15	1.86	1.32	1.25
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	15	1.86	1.32	1.25
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	15	1.86	1.32	1.25
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	15	1.85	0.91	1.53
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	15	1.85	0.91	1.53
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	15	1.85	0.91	1.53
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	15	1.7	1.1	2.03
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	15	1.7	1.1	2.03
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	15	1.7	1.1	2.03
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	15	1.7	1.1	2.03
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	15	1.7	1.1	2.03
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	15	1.7	1.1	2.03
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	15	1.7	1.1	2.03
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	15	1.7	1.1	2.03
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	15	1.7	1.1	2.03
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	15	1.48	0.8	1.18
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	15	1.48	0.8	1.18
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	15	1.48	0.8	1.18
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	15	1.48	0.8	1.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	15	1.48	0.8	1.18
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	15	1.48	0.8	1.18
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	15	1.48	0.8	1.18
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	15	1.48	0.8	1.18
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	15	1.48	0.8	1.18
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	15	1.34	1.17	1.02
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	15	1.34	1.17	1.02
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	15	1.34	1.17	1.02
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	15	1.07	0.16	1.13
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	15	0.85	0.1	0.83
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	14	4.45	1.29	4.46
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	14	4.45	1.29	4.46
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	14	4.45	1.29	4.46
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	14	4.45	1.29	4.46
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	14	4.45	1.29	4.46
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	14	4.45	1.29	4.46
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	14	4.45	1.29	4.46
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	14	4.45	1.29	4.46
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	14	4.45	1.29	4.46
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	14	1.86	0.63	1.71
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	14	1.86	0.63	1.71
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	14	1.86	0.63	1.71
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	14	1.86	0.63	1.71
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	14	1.86	0.63	1.71
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	14	1.86	0.63	1.71
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	14	1.86	0.63	1.71
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	14	1.86	0.63	1.71
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	14	1.86	0.63	1.71
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	14	1.44	1.13	1.11
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	14	1.44	1.13	1.11
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	14	1.44	1.13	1.11
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	13	3.3	1.43	4.24
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	13	3.3	1.43	4.24
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	13	3.3	1.43	4.24
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	13	3.3	1.43	4.24
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	13	3.3	1.43	4.24
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	13	3.3	1.43	4.24
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	13	3.3	1.43	4.24
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	13	3.3	1.43	4.24
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	13	3.3	1.43	4.24
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	13	3.03	1.48	3.0
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	13	3.03	1.48	3.0

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	13	3.03	1.48	3.0
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	13	3.03	1.48	3.0
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	13	3.03	1.48	3.0
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	13	3.03	1.48	3.0
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	13	3.03	1.48	3.0
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	13	3.03	1.48	3.0
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	13	3.03	1.48	3.0
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	13	2.56	1.06	2.44
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	13	2.56	1.06	2.44
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	13	2.56	1.06	2.44
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	13	2.56	1.06	2.44
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	13	2.56	1.06	2.44
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	13	2.56	1.06	2.44
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	13	2.56	1.06	2.44
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	13	2.56	1.06	2.44
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	13	2.56	1.06	2.44
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	13	1.33	1.08	0.88
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	13	1.33	1.08	0.88
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	13	1.33	1.08	0.88
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	13	1.33	1.08	0.88
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	13	1.33	1.08	0.88
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	13	1.33	1.08	0.88
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	13	1.33	1.08	0.88
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	13	1.33	1.08	0.88
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	13	1.33	1.08	0.88
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	13	1.26	0.84	1.41
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	13	1.26	0.84	1.41
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	13	1.26	0.84	1.41
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	12	1.62	0.7	1.46
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	12	1.62	0.7	1.46
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	12	1.62	0.7	1.46
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	12	1.32	0.92	1.22
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	12	1.32	0.92	1.22
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	12	1.32	0.92	1.22
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	12	1.32	0.92	1.22
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	12	1.32	0.92	1.22
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	12	1.32	0.92	1.22
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	12	1.32	0.92	1.22
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	12	1.32	0.92	1.22
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	12	1.32	0.92	1.22
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	12	1.27	0.69	1.1
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	12	1.27	0.69	1.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	12	1.27	0.69	1.1
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	12	1.27	0.69	1.1
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	12	1.27	0.69	1.1
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	12	1.27	0.69	1.1
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	12	1.27	0.69	1.1
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	12	1.27	0.69	1.1
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	12	1.27	0.69	1.1
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	12	1.12	0.71	1.0
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	12	1.12	0.71	1.0
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	12	1.12	0.71	1.0
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	12	1.12	0.71	1.0
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	12	1.12	0.71	1.0
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	12	1.12	0.71	1.0
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	12	1.12	0.71	1.0
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	12	1.12	0.71	1.0
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	12	1.12	0.71	1.0
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	11	2.7	1.36	2.67
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	11	2.7	1.36	2.67
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	11	2.7	1.36	2.67
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	11	2.7	1.36	2.67
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	11	2.7	1.36	2.67
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	11	2.7	1.36	2.67
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	11	2.7	1.36	2.67
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	11	2.7	1.36	2.67
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	11	2.7	1.36	2.67
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	11	2.53	1.79	2.78
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	11	2.53	1.79	2.78
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	11	2.53	1.79	2.78
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	11	2.53	1.79	2.78
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	11	2.53	1.79	2.78
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	11	2.53	1.79	2.78
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	11	2.53	1.79	2.78
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	11	2.53	1.79	2.78
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	11	2.53	1.79	2.78
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	11	1.85	0.88	2.08
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	11	1.85	0.88	2.08
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	11	1.85	0.88	2.08
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	11	1.85	0.88	2.08
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	11	1.85	0.88	2.08
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	11	1.85	0.88	2.08
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	11	1.85	0.88	2.08
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	11	1.85	0.88	2.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	11	1.85	0.88	2.08
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD21	10	2.05	1.3	2.0
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD22	10	2.05	1.3	2.0
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD23	10	2.05	1.3	2.0
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD21	10	2.05	1.3	2.0
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD22	10	2.05	1.3	2.0
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD23	10	2.05	1.3	2.0
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD21	10	2.05	1.3	2.0
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD22	10	2.05	1.3	2.0
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD23	10	2.05	1.3	2.0
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD11	10	1.63	1.14	1.27
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD12	10	1.63	1.14	1.27
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD13	10	1.63	1.14	1.27
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD11	10	1.63	1.14	1.27
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD12	10	1.63	1.14	1.27
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD13	10	1.63	1.14	1.27
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD11	10	1.63	1.14	1.27
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD12	10	1.63	1.14	1.27
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD13	10	1.63	1.14	1.27
(1,351)	1:167:A:LEU:HD11	1:124:A:ILE:H	10	1.34	0.78	1.45
(1,351)	1:167:A:LEU:HD12	1:124:A:ILE:H	10	1.34	0.78	1.45
(1,351)	1:167:A:LEU:HD13	1:124:A:ILE:H	10	1.34	0.78	1.45
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD11	10	1.07	0.85	0.66
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD12	10	1.07	0.85	0.66
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD13	10	1.07	0.85	0.66
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD11	10	1.07	0.85	0.66
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD12	10	1.07	0.85	0.66
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD13	10	1.07	0.85	0.66
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD11	10	1.07	0.85	0.66
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD12	10	1.07	0.85	0.66
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD13	10	1.07	0.85	0.66
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD11	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD12	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD13	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD11	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD12	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD13	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD11	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD12	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD13	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD21	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD22	10	0.98	0.35	1.03

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD23	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD21	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD22	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD23	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD21	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD22	10	0.98	0.35	1.03
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD23	10	0.98	0.35	1.03
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD11	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD12	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD13	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD11	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD12	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD13	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD11	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD12	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD13	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD21	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD22	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD23	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD21	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD22	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD23	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD21	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD22	10	0.98	0.45	1.18
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD23	10	0.98	0.45	1.18
(1,358)	1:176:A:LEU:HD11	1:196:A:TYR:H	9	1.22	0.75	1.39
(1,358)	1:176:A:LEU:HD12	1:196:A:TYR:H	9	1.22	0.75	1.39
(1,358)	1:176:A:LEU:HD13	1:196:A:TYR:H	9	1.22	0.75	1.39
(1,345)	1:163:A:LEU:HD11	1:157:A:LEU:H	9	1.18	0.72	1.02
(1,345)	1:163:A:LEU:HD12	1:157:A:LEU:H	9	1.18	0.72	1.02
(1,345)	1:163:A:LEU:HD13	1:157:A:LEU:H	9	1.18	0.72	1.02
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD11	9	1.03	0.7	0.82
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD12	9	1.03	0.7	0.82
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD13	9	1.03	0.7	0.82
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD11	9	1.03	0.7	0.82
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD12	9	1.03	0.7	0.82
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD13	9	1.03	0.7	0.82
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD11	9	1.03	0.7	0.82
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD12	9	1.03	0.7	0.82
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD13	9	1.03	0.7	0.82
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD21	8	2.82	1.13	3.18
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD22	8	2.82	1.13	3.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD23	8	2.82	1.13	3.18
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD21	8	2.82	1.13	3.18
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD22	8	2.82	1.13	3.18
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD23	8	2.82	1.13	3.18
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD21	8	2.82	1.13	3.18
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD22	8	2.82	1.13	3.18
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD23	8	2.82	1.13	3.18
(1,382)	1:205:A:ILE:HG21	1:216:A:THR:H	8	1.48	0.41	1.55
(1,382)	1:205:A:ILE:HG22	1:216:A:THR:H	8	1.48	0.41	1.55
(1,382)	1:205:A:ILE:HG23	1:216:A:THR:H	8	1.48	0.41	1.55
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG21	8	0.99	0.37	0.99
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG22	8	0.99	0.37	0.99
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG23	8	0.99	0.37	0.99
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG21	8	0.99	0.37	0.99
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG22	8	0.99	0.37	0.99
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG23	8	0.99	0.37	0.99
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG21	8	0.99	0.37	0.99
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG22	8	0.99	0.37	0.99
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG23	8	0.99	0.37	0.99
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG21	8	0.89	0.78	0.55
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG22	8	0.89	0.78	0.55
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG23	8	0.89	0.78	0.55
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG21	8	0.89	0.78	0.55
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG22	8	0.89	0.78	0.55
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG23	8	0.89	0.78	0.55
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG21	8	0.89	0.78	0.55
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG22	8	0.89	0.78	0.55
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG23	8	0.89	0.78	0.55
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD11	8	0.86	0.46	0.78
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD12	8	0.86	0.46	0.78
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD13	8	0.86	0.46	0.78
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD11	8	0.86	0.46	0.78
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD12	8	0.86	0.46	0.78
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD13	8	0.86	0.46	0.78
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD11	8	0.86	0.46	0.78
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD12	8	0.86	0.46	0.78
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD13	8	0.86	0.46	0.78
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD11	8	0.85	0.4	0.86
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD12	8	0.85	0.4	0.86
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD13	8	0.85	0.4	0.86
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD11	8	0.85	0.4	0.86
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD12	8	0.85	0.4	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD13	8	0.85	0.4	0.86
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD11	8	0.85	0.4	0.86
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD12	8	0.85	0.4	0.86
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD13	8	0.85	0.4	0.86
(1,378)	1:195:A:VAL:HG11	1:225:A:ILE:H	8	0.55	0.25	0.48
(1,378)	1:195:A:VAL:HG12	1:225:A:ILE:H	8	0.55	0.25	0.48
(1,378)	1:195:A:VAL:HG13	1:225:A:ILE:H	8	0.55	0.25	0.48
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD11	7	1.2	0.71	1.49
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD12	7	1.2	0.71	1.49
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD13	7	1.2	0.71	1.49
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD11	7	1.2	0.71	1.49
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD12	7	1.2	0.71	1.49
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD13	7	1.2	0.71	1.49
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD11	7	1.2	0.71	1.49
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD12	7	1.2	0.71	1.49
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD13	7	1.2	0.71	1.49
(1,319)	1:89:A:LEU:HD11	1:95:A:ASN:H	7	1.08	0.71	1.14
(1,319)	1:89:A:LEU:HD12	1:95:A:ASN:H	7	1.08	0.71	1.14
(1,319)	1:89:A:LEU:HD13	1:95:A:ASN:H	7	1.08	0.71	1.14
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG11	7	0.99	0.74	0.9
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG12	7	0.99	0.74	0.9
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG13	7	0.99	0.74	0.9
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG11	7	0.99	0.74	0.9
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG12	7	0.99	0.74	0.9
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG13	7	0.99	0.74	0.9
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG11	7	0.99	0.74	0.9
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG12	7	0.99	0.74	0.9
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG13	7	0.99	0.74	0.9
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD21	7	0.84	0.47	0.76
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD22	7	0.84	0.47	0.76
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD23	7	0.84	0.47	0.76
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD21	7	0.84	0.47	0.76
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD22	7	0.84	0.47	0.76
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD23	7	0.84	0.47	0.76
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD21	7	0.84	0.47	0.76
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD22	7	0.84	0.47	0.76
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD23	7	0.84	0.47	0.76
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG21	7	0.6	0.38	0.44
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG22	7	0.6	0.38	0.44
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG23	7	0.6	0.38	0.44
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG21	7	0.6	0.38	0.44
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG22	7	0.6	0.38	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG23	7	0.6	0.38	0.44
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG21	7	0.6	0.38	0.44
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG22	7	0.6	0.38	0.44
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG23	7	0.6	0.38	0.44
(1,352)	1:167:A:LEU:HD21	1:202:A:GLN:H	6	1.81	0.92	2.23
(1,352)	1:167:A:LEU:HD22	1:202:A:GLN:H	6	1.81	0.92	2.23
(1,352)	1:167:A:LEU:HD23	1:202:A:GLN:H	6	1.81	0.92	2.23
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG21	6	1.38	0.56	1.38
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG22	6	1.38	0.56	1.38
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG23	6	1.38	0.56	1.38
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG21	6	1.38	0.56	1.38
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG22	6	1.38	0.56	1.38
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG23	6	1.38	0.56	1.38
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG21	6	1.38	0.56	1.38
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG22	6	1.38	0.56	1.38
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG23	6	1.38	0.56	1.38
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG21	6	0.88	0.68	0.74
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG22	6	0.88	0.68	0.74
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG23	6	0.88	0.68	0.74
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG21	6	0.88	0.68	0.74
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG22	6	0.88	0.68	0.74
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG23	6	0.88	0.68	0.74
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG21	6	0.88	0.68	0.74
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG22	6	0.88	0.68	0.74
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG23	6	0.88	0.68	0.74
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG21	6	0.85	0.65	0.5
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG22	6	0.85	0.65	0.5
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG23	6	0.85	0.65	0.5
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG21	6	0.85	0.65	0.5
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG22	6	0.85	0.65	0.5
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG23	6	0.85	0.65	0.5
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG21	6	0.85	0.65	0.5
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG22	6	0.85	0.65	0.5
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG23	6	0.85	0.65	0.5
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD11	6	0.72	0.26	0.69
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD12	6	0.72	0.26	0.69
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD13	6	0.72	0.26	0.69
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD11	6	0.72	0.26	0.69
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD12	6	0.72	0.26	0.69
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD13	6	0.72	0.26	0.69
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD11	6	0.72	0.26	0.69
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD12	6	0.72	0.26	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD13	6	0.72	0.26	0.69
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG21	6	0.51	0.27	0.48
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG22	6	0.51	0.27	0.48
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG23	6	0.51	0.27	0.48
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG21	6	0.51	0.27	0.48
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG22	6	0.51	0.27	0.48
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG23	6	0.51	0.27	0.48
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG21	6	0.51	0.27	0.48
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG22	6	0.51	0.27	0.48
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG23	6	0.51	0.27	0.48
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG21	5	0.73	0.6	0.47
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG22	5	0.73	0.6	0.47
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG23	5	0.73	0.6	0.47
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG21	5	0.73	0.6	0.47
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG22	5	0.73	0.6	0.47
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG23	5	0.73	0.6	0.47
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG21	5	0.73	0.6	0.47
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG22	5	0.73	0.6	0.47
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG23	5	0.73	0.6	0.47
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD21	5	0.43	0.34	0.29
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD22	5	0.43	0.34	0.29
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD23	5	0.43	0.34	0.29
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD21	5	0.43	0.34	0.29
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD22	5	0.43	0.34	0.29
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD23	5	0.43	0.34	0.29
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD21	5	0.43	0.34	0.29
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD22	5	0.43	0.34	0.29
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD23	5	0.43	0.34	0.29
(1,395)	1:237:A:ILE:HD11	1:228:A:LEU:H	4	1.3	0.75	1.42
(1,395)	1:237:A:ILE:HD12	1:228:A:LEU:H	4	1.3	0.75	1.42
(1,395)	1:237:A:ILE:HD13	1:228:A:LEU:H	4	1.3	0.75	1.42
(1,385)	1:207:A:VAL:HG21	1:162:A:THR:H	4	1.29	0.33	1.16
(1,385)	1:207:A:VAL:HG22	1:162:A:THR:H	4	1.29	0.33	1.16
(1,385)	1:207:A:VAL:HG23	1:162:A:THR:H	4	1.29	0.33	1.16
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD11	4	1.15	0.65	1.09
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD12	4	1.15	0.65	1.09
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD13	4	1.15	0.65	1.09
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD11	4	1.15	0.65	1.09
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD12	4	1.15	0.65	1.09
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD13	4	1.15	0.65	1.09
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD11	4	1.15	0.65	1.09
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD12	4	1.15	0.65	1.09

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD13	4	1.15	0.65	1.09
(1,393)	1:228:A:LEU:HD11	1:238:A:LEU:H	4	0.48	0.09	0.46
(1,393)	1:228:A:LEU:HD12	1:238:A:LEU:H	4	0.48	0.09	0.46
(1,393)	1:228:A:LEU:HD13	1:238:A:LEU:H	4	0.48	0.09	0.46
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD11	4	0.33	0.24	0.26
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD12	4	0.33	0.24	0.26
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD13	4	0.33	0.24	0.26
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD11	4	0.33	0.24	0.26
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD12	4	0.33	0.24	0.26
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD13	4	0.33	0.24	0.26
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD11	4	0.33	0.24	0.26
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD12	4	0.33	0.24	0.26
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD13	4	0.33	0.24	0.26
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB1	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB2	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB3	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB1	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB2	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB3	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB1	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB2	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB3	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB1	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB2	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB3	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB1	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB2	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB3	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB1	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB2	4	0.29	0.1	0.3
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB3	4	0.29	0.1	0.3
(1,396)	1:237:A:ILE:HD11	1:229:A:CYS:H	3	0.76	0.54	0.73
(1,396)	1:237:A:ILE:HD12	1:229:A:CYS:H	3	0.76	0.54	0.73
(1,396)	1:237:A:ILE:HD13	1:229:A:CYS:H	3	0.76	0.54	0.73
(1,324)	1:101:A:LEU:HD11	1:192:A:LEU:HD11	2	0.65	0.46	0.65
(1,324)	1:101:A:LEU:HD11	1:192:A:LEU:HD12	2	0.65	0.46	0.65
(1,324)	1:101:A:LEU:HD11	1:192:A:LEU:HD13	2	0.65	0.46	0.65
(1,324)	1:101:A:LEU:HD12	1:192:A:LEU:HD11	2	0.65	0.46	0.65
(1,324)	1:101:A:LEU:HD12	1:192:A:LEU:HD12	2	0.65	0.46	0.65
(1,324)	1:101:A:LEU:HD12	1:192:A:LEU:HD13	2	0.65	0.46	0.65
(1,324)	1:101:A:LEU:HD13	1:192:A:LEU:HD11	2	0.65	0.46	0.65
(1,324)	1:101:A:LEU:HD13	1:192:A:LEU:HD12	2	0.65	0.46	0.65

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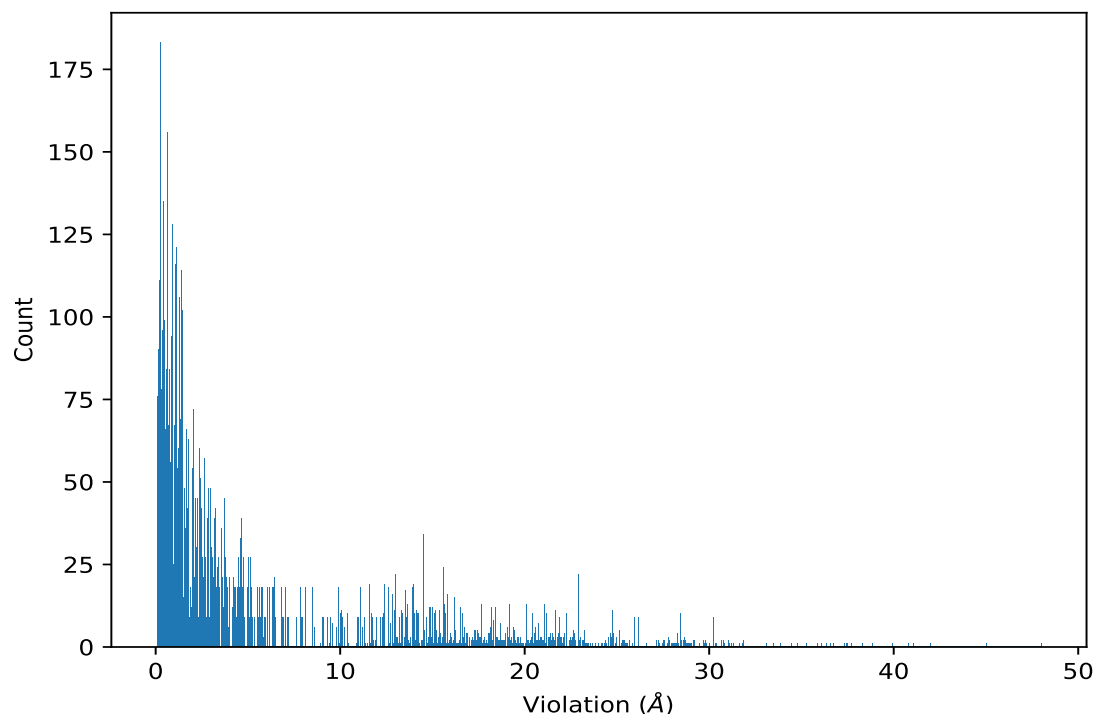
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,324)	1:101:A:LEU:HD13	1:192:A:LEU:HD13	2	0.65	0.46	0.65
(1,386)	1:207:A:VAL:HG21	1:163:A:LEU:HD21	2	0.64	0.26	0.64
(1,386)	1:207:A:VAL:HG21	1:163:A:LEU:HD22	2	0.64	0.26	0.64
(1,386)	1:207:A:VAL:HG21	1:163:A:LEU:HD23	2	0.64	0.26	0.64
(1,386)	1:207:A:VAL:HG22	1:163:A:LEU:HD21	2	0.64	0.26	0.64
(1,386)	1:207:A:VAL:HG22	1:163:A:LEU:HD22	2	0.64	0.26	0.64
(1,386)	1:207:A:VAL:HG22	1:163:A:LEU:HD23	2	0.64	0.26	0.64
(1,386)	1:207:A:VAL:HG23	1:163:A:LEU:HD21	2	0.64	0.26	0.64
(1,386)	1:207:A:VAL:HG23	1:163:A:LEU:HD22	2	0.64	0.26	0.64
(1,386)	1:207:A:VAL:HG23	1:163:A:LEU:HD23	2	0.64	0.26	0.64
(1,344)	1:163:A:LEU:HD21	1:206:A:LYS:H	2	0.56	0.44	0.56
(1,344)	1:163:A:LEU:HD22	1:206:A:LYS:H	2	0.56	0.44	0.56
(1,344)	1:163:A:LEU:HD23	1:206:A:LYS:H	2	0.56	0.44	0.56

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)
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	13	48.03
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	13	45.0
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	1	41.97
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	1	41.09
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	7	40.79
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	5	39.92
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	10	38.88
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	5	38.3
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	9	37.7
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	7	37.47
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	14	37.4
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	10	37.31
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	9	36.74
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	8	36.57
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	14	36.35
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	12	36.06
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	12	35.89
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	8	35.27
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	4	34.78
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	4	34.45
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	15	33.89
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	3	33.48
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	15	33.11
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	8	31.86
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	12	31.85
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	1	31.81
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	9	31.61
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	2	31.34
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	13	31.24
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	7	31.09
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	11	31.04
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	4	31.02
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	5	30.84
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	15	30.78
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	3	30.76
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	10	30.69
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	3	30.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	14	30.35
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	2	30.34
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	13	30.2
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	13	30.2
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	13	30.2
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	13	30.2
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	13	30.2
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	13	30.2
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	13	30.2
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	13	30.2
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	13	30.2
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	6	30.01
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	8	29.86
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	2	29.83
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	12	29.81
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	3	29.74
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	1	29.67
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	9	29.67
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	13	29.48
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	4	29.23
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	7	29.22
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	10	29.16
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	2	29.13
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	11	29.11
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	3	29.04
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	9	28.99
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	1	28.92
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	5	28.89
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	12	28.8
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	9	28.76
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	12	28.74
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	15	28.72
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	15	28.68
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	1	28.68
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	14	28.67
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	6	28.63
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	4	28.6
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	9	28.46
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	6	28.45
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	13	28.43
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	13	28.43
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	13	28.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	13	28.43
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	13	28.43
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	13	28.43
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	13	28.43
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	13	28.43
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	13	28.43
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	3	28.42
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	12	28.3
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	13	28.29
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	5	28.27
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	11	28.26
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	8	28.25
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	4	28.2
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	3	28.19
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	10	28.14
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	13	28.05
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	8	28.02
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	4	27.98
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	7	27.89
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	11	27.85
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	5	27.82
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	2	27.81
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	2	27.79
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	10	27.76
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	6	27.75
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	7	27.73
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	14	27.57
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	15	27.56
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	1	27.51
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	15	27.51
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	10	27.46
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	3	27.3
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	2	27.27
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	7	27.27
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	6	27.12
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	14	27.11
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	5	26.55
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	7	26.16
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	7	26.16
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	7	26.16
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	7	26.16
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	7	26.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	7	26.16
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	7	26.16
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	7	26.16
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	7	26.16
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	7	25.9
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	7	25.9
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	7	25.9
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	7	25.9
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	7	25.9
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	7	25.9
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	7	25.9
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	7	25.9
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	7	25.9
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	1	25.8
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	8	25.69
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	8	25.66
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	3	25.59
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	12	25.51
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	5	25.45
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	3	25.44
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	12	25.41
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	12	25.38
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	1	25.36
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	4	25.33
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	8	25.3
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	9	25.29
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	10	25.26
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	5	25.21
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	11	25.14
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	2	25.12
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	9	25.12
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	10	25.1
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	11	25.1
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	3	24.98
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	7	24.97
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	13	24.95
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	13	24.93
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	2	24.83
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	4	24.83
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	7	24.82
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	2	24.8
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	15	24.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	8	24.77
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	8	24.77
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	8	24.77
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	8	24.77
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	8	24.77
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	8	24.77
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	8	24.77
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	8	24.77
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	8	24.77
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	5	24.77
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	14	24.74
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	15	24.73
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	5	24.71
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	4	24.68
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	12	24.67
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	2	24.64
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	7	24.64
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	7	24.63
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	3	24.62
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	4	24.54
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	6	24.54
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	14	24.54
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	6	24.43
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	15	24.38
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	6	24.38
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	3	24.32
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	6	24.24
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	6	24.15
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	15	24.04
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	4	23.82
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	2	23.65
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	9	23.58
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	12	23.47
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	3	23.44
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	13	23.34
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	1	23.25
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	7	23.23
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	9	23.23
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	10	23.23
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	13	23.21
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	1	23.2
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	4	23.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	4	23.17
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	10	23.13
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	1	23.11
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	8	23.04
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	8	23.01
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	1	23.01
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	8	22.98
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	5	22.95
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	9	22.94
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	1	22.94
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	1	22.93
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	1	22.93
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	1	22.93
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	1	22.93
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	1	22.93
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	1	22.93
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	1	22.93
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	1	22.93
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	1	22.93
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	11	22.93
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	10	22.93
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	8	22.91
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	8	22.91
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	8	22.91
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	8	22.91
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	8	22.91
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	8	22.91
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	8	22.91
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	8	22.91
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	8	22.91
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	3	22.79
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	8	22.77
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	13	22.72
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	11	22.67
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	5	22.67
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	11	22.66
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	8	22.66
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	1	22.64
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	11	22.64
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	11	22.64
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	11	22.62
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	14	22.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	5	22.58
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	12	22.57
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	15	22.56
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	5	22.53
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	8	22.51
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	1	22.49
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	6	22.48
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	6	22.48
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	7	22.4
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	14	22.4
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	1	22.29
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	1	22.29
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	1	22.29
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	1	22.29
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	1	22.29
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	1	22.29
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	1	22.29
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	1	22.29
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	1	22.29
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	14	22.28
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	14	22.19
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	6	22.19
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	13	22.17
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	15	22.16
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	4	22.13
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	3	22.11
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	6	22.1
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	1	22.06
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	13	22.0
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	12	21.96
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	15	21.95
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	12	21.95
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	15	21.93
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	8	21.93
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	10	21.9
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	5	21.89
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	5	21.89
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	5	21.89
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	5	21.89
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	5	21.89
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	5	21.89
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	5	21.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	5	21.89
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	5	21.89
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	13	21.84
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	15	21.83
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	3	21.81
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	2	21.8
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	15	21.78
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	12	21.77
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	12	21.75
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	1	21.68
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	10	21.67
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	10	21.67
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	10	21.67
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	10	21.67
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	10	21.67
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	10	21.67
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	10	21.67
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	10	21.67
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	10	21.67
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	9	21.66
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	3	21.63
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	7	21.63
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	15	21.59
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	14	21.59
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	14	21.55
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	10	21.53
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	5	21.53
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	11	21.53
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	7	21.51
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	1	21.47
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	7	21.47
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	7	21.43
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	14	21.42
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	9	21.38
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	13	21.37
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	7	21.36
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	10	21.35
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	6	21.33
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	9	21.33
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	12	21.3
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	10	21.28
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	10	21.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	13	21.25
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	8	21.19
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	3	21.15
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	3	21.15
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	3	21.15
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	3	21.15
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	3	21.15
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	3	21.15
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	3	21.15
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	3	21.15
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	3	21.15
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	12	21.11
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	14	21.09
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	15	21.08
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	2	21.08
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	13	21.07
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	5	21.05
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	5	21.05
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	5	21.05
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	5	21.05
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	5	21.05
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	5	21.05
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	5	21.05
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	5	21.05
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	5	21.05
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	4	21.0
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	9	21.0
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	15	20.98
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	8	20.96
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	6	20.91
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	6	20.91
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	6	20.91
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	13	20.88
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	12	20.87
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	9	20.86
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	10	20.81
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	8	20.8
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	6	20.79
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	6	20.79
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	5	20.76
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	6	20.74
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	10	20.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:117:A:ASN:H	1:152:A:ALA:H	2	20.73
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	7	20.72
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	7	20.72
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	7	20.72
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	6	20.72
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	3	20.69
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	14	20.69
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	8	20.63
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	11	20.62
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	8	20.59
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	5	20.58
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	9	20.58
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	12	20.56
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	3	20.55
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	15	20.55
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	1	20.53
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	10	20.52
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	5	20.52
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	13	20.52
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	4	20.46
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	9	20.44
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	3	20.41
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	3	20.41
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	3	20.41
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	3	20.41
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	3	20.41
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	3	20.41
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	3	20.41
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	3	20.41
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	3	20.41
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	3	20.38
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	12	20.38
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	11	20.35
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	3	20.33
(1,93)	1:118:A:LYS:H	1:152:A:ALA:H	2	20.3
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	12	20.26
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	14	20.24
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	7	20.24
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	4	20.16
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	9	20.16
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	10	20.14
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	10	20.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	10	20.14
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	10	20.14
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	10	20.14
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	10	20.14
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	10	20.14
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	10	20.14
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	10	20.14
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	15	20.14
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	14	20.1
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	3	20.09
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	14	20.06
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	14	20.06
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	14	20.06
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	14	20.06
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	14	20.06
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	14	20.06
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	14	20.06
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	14	20.06
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	14	20.06
(1,256)	1:199:A:ASP:HA	1:233:A:THR:H	9	20.05
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	4	20.05
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	6	20.05
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	11	20.04
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	7	19.93
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	9	19.88
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	10	19.8
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	15	19.79
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	12	19.79
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	6	19.76
(1,42)	1:123:A:TYR:HA	1:91:A:THR:H	4	19.74
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	4	19.69
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	2	19.69
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	9	19.66
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	5	19.64
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	5	19.61
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	10	19.6
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	4	19.57
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	7	19.53
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	12	19.51
(1,98)	1:152:A:ALA:HA	1:120:A:ILE:H	2	19.46
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	5	19.44
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	1	19.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	4	19.43
(1,257)	1:233:A:THR:H	1:201:A:LYS:H	9	19.41
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	2	19.4
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	2	19.38
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	4	19.37
(1,40)	1:123:A:TYR:H	1:91:A:THR:H	6	19.36
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	14	19.35
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	5	19.35
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	13	19.35
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	14	19.33
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	7	19.28
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	2	19.27
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	7	19.26
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	11	19.24
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	11	19.2
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	3	19.18
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	2	19.17
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	10	19.17
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	9	19.16
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	9	19.16
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	9	19.16
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	9	19.16
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	9	19.16
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	9	19.16
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	9	19.16
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	9	19.16
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	9	19.16
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	13	19.15
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	3	19.11
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	3	19.11
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	3	19.11
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	3	19.08
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	1	19.07
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	15	19.06
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	15	19.06
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	4	19.06
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	6	19.05
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	7	18.98
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	4	18.98
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	1	18.97
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	14	18.96
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	8	18.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	8	18.93
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	13	18.89
(1,117)	1:126:A:VAL:H	1:160:A:ASN:H	1	18.85
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	8	18.81
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	14	18.78
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	8	18.75
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	7	18.72
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	6	18.71
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	6	18.69
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	1	18.69
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	1	18.68
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	6	18.68
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	1	18.67
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	14	18.66
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	11	18.65
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	3	18.63
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	10	18.6
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	9	18.56
(1,115)	1:125:A:ASN:H	1:160:A:ASN:H	13	18.56
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	9	18.51
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	6	18.51
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	14	18.51
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	8	18.48
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	2	18.45
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	11	18.45
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	12	18.44
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	9	18.44
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	4	18.43
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	15	18.42
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	10	18.42
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	5	18.41
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	5	18.41
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	5	18.41
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	12	18.4
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	12	18.4
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	12	18.4
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	3	18.4
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	1	18.34
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	15	18.34
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	2	18.32
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	2	18.32
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	2	18.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	15	18.32
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	12	18.31
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	13	18.3
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	11	18.27
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	7	18.26
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	13	18.24
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	10	18.24
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	5	18.24
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	14	18.19
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	14	18.19
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	14	18.19
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	14	18.19
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	14	18.19
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	14	18.19
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	14	18.19
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	14	18.19
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	14	18.19
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	11	18.19
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	11	18.18
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	3	18.16
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	14	18.14
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	15	18.13
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	15	18.13
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	15	18.13
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	12	18.12
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	5	18.12
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	3	18.08
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	4	18.05
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	4	18.05
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	4	18.05
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	5	18.04
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	7	18.04
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	7	18.02
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	1	18.01
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	1	17.97
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	8	17.91
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	11	17.9
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	2	17.89
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	9	17.83
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	9	17.82
(1,95)	1:118:A:LYS:HA	1:152:A:ALA:H	2	17.8
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	12	17.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	13	17.77
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	15	17.71
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	14	17.68
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	12	17.68
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	8	17.67
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	14	17.67
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	9	17.65
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	9	17.65
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	9	17.65
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	9	17.65
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	9	17.65
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	9	17.65
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	9	17.65
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	9	17.65
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	9	17.65
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	10	17.62
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	14	17.61
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	14	17.6
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	4	17.56
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	7	17.54
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	2	17.51
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	10	17.5
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	8	17.47
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	6	17.46
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	4	17.46
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	11	17.45
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	1	17.44
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	7	17.43
(1,37)	1:89:A:LEU:H	1:123:A:TYR:H	15	17.42
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	13	17.41
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	15	17.4
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	4	17.38
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	8	17.35
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	10	17.34
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	13	17.33
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	14	17.32
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	15	17.31
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	6	17.3
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	9	17.29
(1,96)	1:152:A:ALA:H	1:120:A:ILE:H	2	17.29
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	6	17.29
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	6	17.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	3	17.27
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	5	17.23
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	1	17.22
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	12	17.19
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	4	17.19
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	7	17.18
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	10	17.14
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	3	17.14
(1,41)	1:123:A:TYR:H	1:92:A:PHE:H	2	17.03
(1,35)	1:88:A:ARG:H	1:123:A:TYR:H	15	17.03
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	13	17.0
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	10	16.93
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	2	16.9
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	2	16.9
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	8	16.88
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	9	16.86
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	15	16.85
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	7	16.85
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	11	16.84
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	1	16.83
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	8	16.83
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	9	16.8
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	3	16.76
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	6	16.73
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	13	16.72
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	11	16.72
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	7	16.72
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	8	16.71
(1,296)	1:225:A:ILE:HA	1:259:A:ALA:H	5	16.7
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	5	16.67
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	12	16.65
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	11	16.65
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	15	16.61
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	15	16.61
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	15	16.61
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	15	16.61
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	15	16.61
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	15	16.61
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	15	16.61
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	15	16.61
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	15	16.61
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	1	16.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	15	16.57
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	3	16.54
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	3	16.54
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	3	16.54
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	3	16.54
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	3	16.54
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	3	16.54
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	8	16.53
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	8	16.53
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	8	16.53
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	12	16.53
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	14	16.52
(1,297)	1:259:A:ALA:H	1:227:A:PHE:H	5	16.5
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	9	16.49
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	2	16.46
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	2	16.44
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	4	16.39
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	1	16.3
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	11	16.29
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	7	16.26
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	11	16.26
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	7	16.25
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	5	16.25
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	15	16.24
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	15	16.23
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	7	16.22
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	4	16.2
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	1	16.19
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	1	16.19
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	1	16.19
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	6	16.19
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	14	16.19
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	15	16.19
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	3	16.16
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	3	16.16
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	3	16.16
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	3	16.16
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	3	16.16
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	3	16.16
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	3	16.16
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	3	16.16
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	3	16.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	4	16.11
(1,119)	1:126:A:VAL:HA	1:160:A:ASN:H	13	16.11
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	2	16.06
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	9	16.03
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	10	16.02
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	11	16.01
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	14	15.99
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	9	15.97
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	14	15.96
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	11	15.95
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	5	15.93
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	7	15.9
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	6	15.85
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	10	15.84
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	15	15.83
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	7	15.83
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	14	15.82
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	1	15.82
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	15	15.81
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	15	15.81
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	15	15.81
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	15	15.81
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	15	15.81
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	15	15.81
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	15	15.81
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	15	15.81
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	15	15.81
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	11	15.81
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	13	15.8
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	10	15.78
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	3	15.74
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	3	15.7
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	3	15.7
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	3	15.7
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	3	15.7
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	3	15.7
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	3	15.7
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	3	15.7
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	3	15.7
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	3	15.7
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	8	15.69
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	12	15.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	12	15.68
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	12	15.68
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	12	15.68
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	12	15.68
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	12	15.68
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	12	15.68
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	12	15.68
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	12	15.68
(1,120)	1:160:A:ASN:H	1:128:A:THR:H	13	15.67
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	8	15.66
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	14	15.65
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	7	15.64
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	4	15.63
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	4	15.63
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	4	15.63
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	4	15.63
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	4	15.63
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	4	15.63
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	4	15.63
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	4	15.63
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	4	15.63
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	13	15.61
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	10	15.59
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	10	15.59
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	10	15.59
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	10	15.59
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	10	15.59
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	10	15.59
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	10	15.59
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	10	15.59
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	10	15.59
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	6	15.57
(1,39)	1:89:A:LEU:HA	1:123:A:TYR:H	15	15.57
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	11	15.56
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	11	15.56
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	11	15.56
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	5	15.56
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	5	15.56
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	5	15.56
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	5	15.56
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	5	15.56
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	5	15.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	5	15.56
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	5	15.56
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	5	15.56
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	3	15.55
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	2	15.54
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	2	15.53
(1,97)	1:152:A:ALA:H	1:121:A:GLU:H	2	15.53
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	1	15.49
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	4	15.43
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	10	15.43
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	1	15.42
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	11	15.41
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	12	15.39
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	12	15.38
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	13	15.35
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	13	15.35
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	13	15.35
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	13	15.35
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	13	15.35
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	13	15.35
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	13	15.35
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	13	15.35
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	13	15.35
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	13	15.33
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	13	15.33
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	13	15.33
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	6	15.29
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	14	15.24
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	2	15.21
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	9	15.2
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	9	15.2
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	9	15.2
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	5	15.17
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	15	15.15
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	15	15.15
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	15	15.15
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	15	15.15
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	15	15.15
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	15	15.15
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	15	15.15
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	15	15.15
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	15	15.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	8	15.15
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	10	15.14
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	10	15.14
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	10	15.14
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	15	15.12
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	15	15.12
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	15	15.12
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	15	15.12
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	15	15.12
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	15	15.12
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	14	15.11
(1,255)	1:199:A:ASP:H	1:233:A:THR:H	9	15.09
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	6	15.04
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	14	15.03
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	14	15.03
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	14	15.03
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	14	15.03
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	14	15.03
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	14	15.03
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	14	15.03
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	14	15.03
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	14	15.03
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	14	15.02
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	8	15.02
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	11	14.99
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	5	14.97
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	11	14.95
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	9	14.93
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	7	14.86
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	7	14.86
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	7	14.86
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	7	14.86
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	7	14.86
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	7	14.86
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	7	14.86
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	7	14.86
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	7	14.86
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	8	14.85
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	1	14.85
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	3	14.85
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	4	14.84
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	7	14.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	7	14.81
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	7	14.81
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	7	14.81
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	7	14.81
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	7	14.81
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	7	14.81
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	7	14.81
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	7	14.81
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	9	14.81
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	3	14.81
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	1	14.78
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	12	14.78
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	8	14.75
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	15	14.74
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	8	14.68
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	8	14.68
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	8	14.68
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	8	14.68
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	8	14.68
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	8	14.68
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	8	14.68
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	8	14.68
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	8	14.68
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	10	14.57
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	11	14.56
(1,380)	1:233:A:THR:HG21	1:168:A:ILE:H	14	14.55
(1,380)	1:233:A:THR:HG22	1:168:A:ILE:H	14	14.55
(1,380)	1:233:A:THR:HG23	1:168:A:ILE:H	14	14.55
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	1	14.54
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	1	14.54
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	1	14.54
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	1	14.54
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	1	14.54
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	1	14.54
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	1	14.54
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	1	14.54
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	1	14.54
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	9	14.54
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	9	14.54
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	9	14.54
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	9	14.54
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	9	14.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	9	14.54
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	9	14.54
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	9	14.54
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	9	14.54
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	2	14.52
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	2	14.52
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	2	14.52
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	2	14.52
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	2	14.52
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	2	14.52
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	2	14.52
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	2	14.52
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	2	14.52
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	12	14.52
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	9	14.5
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	9	14.5
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	9	14.5
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	9	14.5
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	9	14.5
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	9	14.5
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	9	14.48
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	8	14.47
(1,158)	1:180:A:GLN:H	1:148:A:GLU:H	11	14.44
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	11	14.4
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	2	14.27
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	13	14.23
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	12	14.21
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	12	14.21
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	12	14.21
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	12	14.21
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	12	14.21
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	12	14.21
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	12	14.21
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	12	14.21
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	12	14.21
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	13	14.18
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	6	14.15
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	6	14.15
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	6	14.15
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	6	14.15
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	6	14.15
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	6	14.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	6	14.15
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	6	14.15
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	6	14.15
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	9	14.13
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	2	14.11
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	2	14.11
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	2	14.11
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	2	14.11
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	2	14.11
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	2	14.11
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	2	14.11
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	2	14.11
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	2	14.11
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	4	14.11
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	7	14.05
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	13	14.05
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	11	14.04
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	11	14.04
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	11	14.04
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	11	14.04
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	11	14.04
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	11	14.04
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	11	14.04
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	11	14.04
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	11	14.04
(1,122)	1:160:A:ASN:HA	1:128:A:THR:H	13	14.02
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	12	13.99
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	12	13.99
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	12	13.99
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	12	13.99
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	12	13.99
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	12	13.99
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	12	13.99
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	12	13.99
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	12	13.99
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	9	13.97
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	9	13.97
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	9	13.97
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	9	13.97
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	9	13.97
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	9	13.97
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	9	13.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	9	13.97
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	9	13.97
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	3	13.95
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	4	13.9
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	4	13.9
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	4	13.9
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	4	13.9
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	4	13.9
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	4	13.9
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	4	13.9
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	4	13.9
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	4	13.9
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	1	13.9
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	1	13.9
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	1	13.9
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	1	13.9
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	1	13.9
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	1	13.9
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	1	13.9
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	1	13.9
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	1	13.9
(1,156)	1:179:A:VAL:H	1:148:A:GLU:H	6	13.83
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	3	13.8
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	2	13.8
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	5	13.78
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	5	13.72
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	11	13.7
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	1	13.67
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	3	13.63
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	9	13.63
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	3	13.63
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	2	13.62
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	6	13.61
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	6	13.61
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	6	13.61
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	6	13.61
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	6	13.61
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	6	13.61
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	6	13.61
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	6	13.61
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	6	13.61
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	6	13.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	6	13.56
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	6	13.56
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	6	13.56
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	6	13.56
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	6	13.56
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	6	13.56
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	6	13.56
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	6	13.56
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	7	13.54
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	7	13.54
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	7	13.54
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	7	13.54
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	7	13.54
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	7	13.54
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	7	13.54
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	7	13.54
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	7	13.54
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	12	13.52
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	12	13.52
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	12	13.52
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	12	13.52
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	12	13.52
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	12	13.52
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	5	13.51
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	10	13.51
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	10	13.49
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	7	13.46
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	10	13.45
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	5	13.38
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	4	13.37
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	4	13.37
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	4	13.37
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	4	13.37
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	4	13.37
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	4	13.37
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	4	13.37
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	4	13.37
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	4	13.37
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	10	13.33
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	4	13.33
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	12	13.31
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	12	13.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	12	13.31
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	12	13.31
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	12	13.31
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	12	13.31
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	12	13.31
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	12	13.31
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	12	13.31
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	14	13.27
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	2	13.2
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	2	13.2
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	2	13.2
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	2	13.2
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	2	13.2
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	2	13.2
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	2	13.2
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	2	13.2
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	2	13.2
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	4	13.16
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	10	13.12
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	12	13.1
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	5	13.1
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	2	13.07
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	1	13.06
(1,121)	1:160:A:ASN:H	1:129:A:SER:H	13	13.06
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB1	15	13.04
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB2	15	13.04
(1,361)	1:177:A:VAL:HG21	1:152:A:ALA:HB3	15	13.04
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB1	15	13.04
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB2	15	13.04
(1,361)	1:177:A:VAL:HG22	1:152:A:ALA:HB3	15	13.04
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB1	15	13.04
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB2	15	13.04
(1,361)	1:177:A:VAL:HG23	1:152:A:ALA:HB3	15	13.04
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	8	13.02
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	8	13.02
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	8	13.02
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	8	13.02
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	8	13.02
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	8	13.02
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	2	13.01
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	2	13.01
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	2	13.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	2	13.01
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	2	13.01
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	2	13.01
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	13	13.0
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	3	12.96
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	12	12.93
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	12	12.9
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	12	12.9
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	12	12.9
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	12	12.9
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	12	12.9
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	12	12.9
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	12	12.9
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	12	12.9
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	12	12.9
(1,160)	1:180:A:GLN:HA	1:148:A:GLU:H	5	12.9
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	4	12.85
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	6	12.83
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	6	12.83
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	6	12.83
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	6	12.83
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	6	12.83
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	6	12.83
(1,154)	1:145:A:TRP:HA	1:179:A:VAL:H	6	12.83
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	5	12.8
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	5	12.8
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	5	12.8
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	5	12.8
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	5	12.8
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	5	12.8
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	5	12.8
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	5	12.8
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	5	12.8
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	5	12.72
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	1	12.71
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	1	12.71
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	1	12.71
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	1	12.71
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	1	12.71
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	1	12.71
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	8	12.67
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	6	12.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	6	12.64
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	6	12.64
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	6	12.64
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	6	12.64
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	6	12.64
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	6	12.64
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	6	12.64
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	6	12.64
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	3	12.61
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	3	12.61
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	3	12.61
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	3	12.61
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	3	12.61
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	3	12.61
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	3	12.61
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	3	12.61
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	3	12.61
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	8	12.43
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	8	12.43
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	8	12.43
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	8	12.43
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	8	12.43
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	8	12.43
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	8	12.43
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	8	12.43
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	8	12.43
(1,159)	1:180:A:GLN:H	1:149:A:ALA:H	11	12.42
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	8	12.41
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	8	12.41
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	8	12.41
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	8	12.41
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	8	12.41
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	8	12.41
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	8	12.41
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	8	12.41
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	8	12.41
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	10	12.38
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	10	12.38
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	10	12.38
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	10	12.38
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	10	12.38
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	10	12.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	2	12.31
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	2	12.31
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	2	12.31
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	2	12.31
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	2	12.31
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	2	12.31
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	2	12.31
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	2	12.31
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	2	12.31
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	12	12.3
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	15	12.27
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	15	12.27
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	15	12.27
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	15	12.27
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	15	12.27
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	15	12.27
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	15	12.27
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	15	12.27
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	15	12.27
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	2	12.16
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	2	12.16
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	2	12.16
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	2	12.16
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	2	12.16
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	2	12.16
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	2	12.16
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	2	12.16
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	2	12.16
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	1	11.99
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	1	11.99
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	1	11.99
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	1	11.99
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	1	11.99
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	1	11.99
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	1	11.99
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	1	11.99
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	1	11.99
(1,295)	1:225:A:ILE:H	1:259:A:ALA:H	13	11.93
(1,152)	1:145:A:TRP:H	1:179:A:VAL:H	6	11.92
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	4	11.84
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	13	11.83
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	9	11.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	9	11.77
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	9	11.77
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	9	11.77
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	9	11.77
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	9	11.77
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	9	11.77
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	9	11.77
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	9	11.77
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	7	11.73
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	7	11.73
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	7	11.73
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	7	11.73
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	7	11.73
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	7	11.73
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	10	11.68
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	10	11.68
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	10	11.68
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	10	11.68
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	10	11.68
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	10	11.68
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	10	11.68
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	10	11.68
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	10	11.68
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	15	11.66
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	4	11.61
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	10	11.58
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	10	11.58
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	10	11.58
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	10	11.58
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	10	11.58
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	10	11.58
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	10	11.58
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	10	11.58
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	10	11.58
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	10	11.57
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	4	11.56
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	4	11.56
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	4	11.56
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	4	11.56
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	4	11.56
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	4	11.56
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	4	11.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	4	11.56
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	4	11.56
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	12	11.45
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	6	11.36
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	3	11.3
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	3	11.3
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	3	11.3
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	3	11.3
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	3	11.3
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	3	11.3
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	3	11.3
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	3	11.3
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	3	11.3
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	4	11.22
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	4	11.22
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	4	11.22
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	4	11.22
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	4	11.22
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	4	11.22
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	11	11.09
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	11	11.09
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	11	11.09
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	11	11.09
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	11	11.09
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	11	11.09
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	11	11.09
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	11	11.09
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	11	11.09
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	2	11.05
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	2	11.05
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	2	11.05
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	2	11.05
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	2	11.05
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	2	11.05
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	2	11.05
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	2	11.05
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	2	11.05
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	7	10.95
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	7	10.95
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	7	10.95
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	7	10.95
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	7	10.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	7	10.95
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	7	10.95
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	7	10.95
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	7	10.95
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	5	10.94
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	5	10.94
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	5	10.94
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	5	10.94
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	5	10.94
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	5	10.94
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	5	10.94
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	5	10.94
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	5	10.94
(1,150)	1:144:A:LEU:H	1:179:A:VAL:H	6	10.86
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	7	10.48
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	12	10.38
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	13	10.36
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	13	10.36
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	13	10.36
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	13	10.36
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	13	10.36
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	13	10.36
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	13	10.36
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	13	10.36
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	13	10.36
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	14	10.22
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	14	10.22
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	14	10.22
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	14	10.22
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	14	10.22
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	14	10.22
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	4	10.13
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	4	10.13
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	4	10.13
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	4	10.13
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	4	10.13
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	4	10.13
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	4	10.13
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	4	10.13
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	4	10.13
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	9	10.09
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	12	10.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	12	10.08
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	12	10.08
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	12	10.08
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	12	10.08
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	12	10.08
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	12	10.08
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	12	10.08
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	12	10.08
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	14	10.07
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	3	10.03
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	13	10.0
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	13	10.0
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	13	10.0
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	13	10.0
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	13	10.0
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	13	10.0
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	13	10.0
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	13	10.0
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	13	10.0
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	2	9.96
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	4	9.94
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	4	9.94
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	4	9.94
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	4	9.94
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	4	9.94
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	4	9.94
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	4	9.94
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	4	9.94
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	4	9.94
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	6	9.93
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	6	9.93
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	6	9.93
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	6	9.93
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	6	9.93
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	6	9.93
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	6	9.93
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	6	9.93
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	6	9.93
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	13	9.8
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	13	9.8
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	13	9.8
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	13	9.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	13	9.8
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	13	9.8
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	11	9.58
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	11	9.58
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	11	9.58
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	11	9.58
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	11	9.58
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	11	9.58
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	8	9.56
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	15	9.45
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	15	9.45
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	15	9.45
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	15	9.45
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	15	9.45
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	15	9.45
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	15	9.45
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	15	9.45
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	15	9.45
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	5	9.44
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	14	9.3
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	14	9.3
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	14	9.3
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	14	9.3
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	14	9.3
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	14	9.3
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	14	9.3
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	14	9.3
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	14	9.3
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	1	9.08
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	1	9.08
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	1	9.08
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	1	9.08
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	1	9.08
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	1	9.08
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	1	9.08
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	1	9.08
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	1	9.08
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG21	14	9.03
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG22	14	9.03
(1,349)	1:167:A:LEU:HD21	1:233:A:THR:HG23	14	9.03
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG21	14	9.03
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG22	14	9.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:167:A:LEU:HD22	1:233:A:THR:HG23	14	9.03
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG21	14	9.03
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG22	14	9.03
(1,349)	1:167:A:LEU:HD23	1:233:A:THR:HG23	14	9.03
(1,153)	1:145:A:TRP:H	1:180:A:GLN:H	11	8.94
(1,377)	1:195:A:VAL:HG21	1:259:A:ALA:H	5	8.63
(1,377)	1:195:A:VAL:HG22	1:259:A:ALA:H	5	8.63
(1,377)	1:195:A:VAL:HG23	1:259:A:ALA:H	5	8.63
(1,373)	1:195:A:VAL:HG21	1:259:A:ALA:H	5	8.63
(1,373)	1:195:A:VAL:HG22	1:259:A:ALA:H	5	8.63
(1,373)	1:195:A:VAL:HG23	1:259:A:ALA:H	5	8.63
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	5	8.53
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	5	8.53
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	5	8.53
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	5	8.53
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	5	8.53
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	5	8.53
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	5	8.53
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	5	8.53
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	5	8.53
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	15	8.5
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	15	8.5
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	15	8.5
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	15	8.5
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	15	8.5
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	15	8.5
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	15	8.5
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	15	8.5
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	15	8.5
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	11	8.14
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	11	8.14
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	11	8.14
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	11	8.14
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	11	8.14
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	11	8.14
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	11	8.14
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	11	8.14
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	11	8.14
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB1	5	8.13
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB2	5	8.13
(1,374)	1:195:A:VAL:HG21	1:259:A:ALA:HB3	5	8.13
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB1	5	8.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB2	5	8.13
(1,374)	1:195:A:VAL:HG22	1:259:A:ALA:HB3	5	8.13
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB1	5	8.13
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB2	5	8.13
(1,374)	1:195:A:VAL:HG23	1:259:A:ALA:HB3	5	8.13
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	14	7.96
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	14	7.96
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	14	7.96
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	14	7.96
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	14	7.96
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	14	7.96
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	14	7.96
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	14	7.96
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	14	7.96
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	6	7.91
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	6	7.91
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	6	7.91
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	6	7.91
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	6	7.91
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	6	7.91
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	6	7.91
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	6	7.91
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	6	7.91
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	13	7.89
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	13	7.89
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	13	7.89
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	13	7.89
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	13	7.89
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	13	7.89
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	13	7.89
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	13	7.89
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	13	7.89
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	2	7.87
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	2	7.87
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	2	7.87
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	2	7.87
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	2	7.87
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	2	7.87
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	2	7.87
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	2	7.87
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	2	7.87
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	3	7.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	3	7.83
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	3	7.83
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	3	7.83
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	3	7.83
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	3	7.83
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	3	7.83
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	3	7.83
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	3	7.83
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	8	7.63
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	8	7.63
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	8	7.63
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	8	7.63
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	8	7.63
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	8	7.63
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	8	7.63
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	8	7.63
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	8	7.63
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	13	7.22
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	13	7.22
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	13	7.22
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	13	7.22
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	13	7.22
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	13	7.22
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	13	7.22
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	13	7.22
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	13	7.22
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	10	7.17
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	10	7.17
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	10	7.17
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	10	7.17
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	10	7.17
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	10	7.17
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	10	7.17
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	10	7.17
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	10	7.17
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	7	7.1
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	7	7.1
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	7	7.1
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	7	7.1
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	7	7.1
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	7	7.1
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	7	7.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	7	7.1
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	7	7.1
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	10	7.04
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	10	7.04
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	10	7.04
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	10	7.04
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	10	7.04
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	10	7.04
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	10	7.04
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	10	7.04
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	10	7.04
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	1	7.02
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	1	7.02
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	1	7.02
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	1	7.02
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	1	7.02
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	1	7.02
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	1	7.02
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	1	7.02
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	1	7.02
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	14	6.9
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	14	6.9
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	14	6.9
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	14	6.9
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	14	6.9
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	14	6.9
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	14	6.9
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	14	6.9
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	14	6.9
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	10	6.89
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	10	6.89
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	10	6.89
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	10	6.89
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	10	6.89
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	10	6.89
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	10	6.89
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	10	6.89
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	10	6.89
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	12	6.84
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	12	6.84
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	12	6.84
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	12	6.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	12	6.84
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	12	6.84
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	12	6.84
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	12	6.84
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	12	6.84
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	11	6.8
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	11	6.8
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	11	6.8
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	11	6.8
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	11	6.8
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	11	6.8
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	11	6.8
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	11	6.8
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	11	6.8
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	8	6.48
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	8	6.48
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	8	6.48
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	8	6.48
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	8	6.48
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	8	6.48
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	8	6.48
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	8	6.48
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	8	6.48
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	6	6.44
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	6	6.44
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	6	6.44
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	6	6.44
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	6	6.44
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	6	6.44
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	6	6.44
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	6	6.44
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	6	6.44
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	10	6.43
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	10	6.43
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	10	6.43
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	10	6.43
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	10	6.43
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	10	6.43
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	10	6.43
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	10	6.43
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	10	6.43
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	3	6.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	3	6.42
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	3	6.42
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	9	6.39
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	9	6.39
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	9	6.39
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	9	6.39
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	9	6.39
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	9	6.39
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	9	6.39
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	9	6.39
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	9	6.39
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	8	6.38
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	8	6.38
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	8	6.38
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	8	6.38
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	8	6.38
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	8	6.38
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	8	6.38
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	8	6.38
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	8	6.38
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	11	6.33
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	11	6.33
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	11	6.33
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	11	6.33
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	11	6.33
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	11	6.33
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	11	6.33
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	11	6.33
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	11	6.33
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	1	6.3
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	1	6.3
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	1	6.3
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	1	6.3
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	1	6.3
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	1	6.3
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	1	6.3
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	1	6.3
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	1	6.3
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	3	6.19
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	3	6.19
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	3	6.19
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	3	6.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	3	6.19
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	3	6.19
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	3	6.19
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	3	6.19
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	3	6.19
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	13	6.18
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	13	6.18
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	13	6.18
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	13	6.18
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	13	6.18
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	13	6.18
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	13	6.18
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	13	6.18
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	13	6.18
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	9	6.09
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	9	6.09
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	9	6.09
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	9	6.09
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	9	6.09
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	9	6.09
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	9	6.09
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	9	6.09
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	9	6.09
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	9	6.06
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	9	6.06
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	9	6.06
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	9	6.06
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	9	6.06
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	9	6.06
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	9	6.06
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	9	6.06
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	9	6.06
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	2	5.95
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	2	5.95
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	2	5.95
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	2	5.95
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	2	5.95
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	2	5.95
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	2	5.95
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	2	5.95
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	2	5.95
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	8	5.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	8	5.85
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	8	5.85
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	8	5.85
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	8	5.85
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	8	5.85
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	8	5.85
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	8	5.85
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	8	5.85
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	6	5.8
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	6	5.8
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	6	5.8
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	4	5.79
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	4	5.79
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	4	5.79
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	4	5.79
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	4	5.79
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	4	5.79
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	4	5.79
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	4	5.79
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	4	5.79
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD11	14	5.76
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD12	14	5.76
(1,379)	1:233:A:THR:HG21	1:120:A:ILE:HD13	14	5.76
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD11	14	5.76
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD12	14	5.76
(1,379)	1:233:A:THR:HG22	1:120:A:ILE:HD13	14	5.76
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD11	14	5.76
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD12	14	5.76
(1,379)	1:233:A:THR:HG23	1:120:A:ILE:HD13	14	5.76
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	5	5.71
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	5	5.71
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	5	5.71
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	5	5.71
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	5	5.71
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	5	5.71
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	5	5.71
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	5	5.71
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	5	5.71
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	2	5.71
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	2	5.71
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	2	5.71
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	2	5.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	2	5.71
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	2	5.71
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	2	5.71
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	2	5.71
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	2	5.71
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	7	5.69
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	7	5.69
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	7	5.69
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	7	5.69
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	7	5.69
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	7	5.69
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	7	5.69
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	7	5.69
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	7	5.69
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	7	5.62
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	7	5.62
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	7	5.62
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	7	5.62
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	7	5.62
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	7	5.62
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	7	5.62
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	7	5.62
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	7	5.62
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	5	5.62
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	5	5.62
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	5	5.62
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	5	5.62
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	5	5.62
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	5	5.62
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	5	5.62
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	5	5.62
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	5	5.62
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	13	5.58
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	13	5.58
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	13	5.58
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	13	5.58
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	13	5.58
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	13	5.58
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	13	5.58
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	13	5.58
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	13	5.58
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	9	5.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	9	5.51
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	9	5.51
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	9	5.51
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	9	5.51
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	9	5.51
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	9	5.51
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	9	5.51
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	9	5.51
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	3	5.5
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	3	5.5
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	3	5.5
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	3	5.5
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	3	5.5
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	3	5.5
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	3	5.5
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	3	5.5
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	3	5.5
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	7	5.39
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	7	5.39
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	7	5.39
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	7	5.39
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	7	5.39
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	7	5.39
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	7	5.39
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	7	5.39
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	7	5.39
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	13	5.26
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	13	5.26
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	13	5.26
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	13	5.26
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	13	5.26
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	13	5.26
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	13	5.26
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	13	5.26
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	13	5.26
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	12	5.2
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	12	5.2
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	12	5.2
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	12	5.2
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	12	5.2
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	12	5.2
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	12	5.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	12	5.2
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	12	5.2
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	1	5.19
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	1	5.19
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	1	5.19
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	1	5.19
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	1	5.19
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	1	5.19
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	1	5.19
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	1	5.19
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	1	5.19
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	4	5.18
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	4	5.18
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	4	5.18
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	4	5.18
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	4	5.18
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	4	5.18
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	4	5.18
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	4	5.18
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	4	5.18
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	6	5.13
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	6	5.13
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	6	5.13
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	6	5.13
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	6	5.13
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	6	5.13
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	6	5.13
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	6	5.13
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	6	5.13
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	12	5.13
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	12	5.13
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	12	5.13
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	12	5.13
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	12	5.13
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	12	5.13
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	12	5.13
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	12	5.13
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	12	5.13
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	4	5.12
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	4	5.12
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	4	5.12
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	4	5.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	4	5.12
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	4	5.12
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	4	5.12
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	4	5.12
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	4	5.12
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	3	5.08
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	3	5.08
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	3	5.08
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	3	5.08
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	3	5.08
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	3	5.08
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	3	5.08
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	3	5.08
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	3	5.08
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	12	5.04
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	12	5.04
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	12	5.04
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	12	5.04
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	12	5.04
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	12	5.04
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	12	5.04
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	12	5.04
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	12	5.04
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	14	5.03
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	14	5.03
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	14	5.03
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	14	5.03
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	14	5.03
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	14	5.03
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	14	5.03
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	14	5.03
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	14	5.03
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	1	5.03
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	1	5.03
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	1	5.03
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	1	5.03
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	1	5.03
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	1	5.03
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	1	5.03
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	1	5.03
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	1	5.03
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	10	4.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	10	4.95
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	10	4.95
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	10	4.95
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	10	4.95
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	10	4.95
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	10	4.95
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	10	4.95
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	10	4.95
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	11	4.95
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	11	4.95
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	11	4.95
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	11	4.95
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	11	4.95
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	11	4.95
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	11	4.95
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	11	4.95
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	11	4.95
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	5	4.81
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	5	4.81
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	5	4.81
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	5	4.81
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	5	4.81
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	5	4.81
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	5	4.81
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	5	4.81
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	5	4.81
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	6	4.78
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	6	4.78
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	6	4.78
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	6	4.78
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	6	4.78
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	6	4.78
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	6	4.78
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	6	4.78
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	6	4.78
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	13	4.76
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	13	4.76
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	13	4.76
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	13	4.76
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	13	4.76
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	13	4.76
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	13	4.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	13	4.76
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	13	4.76
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	10	4.75
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	10	4.75
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	10	4.75
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	10	4.75
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	10	4.75
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	10	4.75
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	10	4.75
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	10	4.75
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	10	4.75
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	6	4.74
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	6	4.74
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	6	4.74
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	6	4.74
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	6	4.74
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	6	4.74
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	6	4.74
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	6	4.74
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	6	4.74
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	12	4.73
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	12	4.73
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	12	4.73
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	12	4.73
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	12	4.73
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	12	4.73
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	12	4.73
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	12	4.73
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	12	4.73
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	4	4.69
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	4	4.69
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	4	4.69
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	4	4.69
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	4	4.69
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	4	4.69
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	4	4.69
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	4	4.69
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	4	4.69
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	4	4.69
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	4	4.69
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	4	4.69
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	4	4.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	4	4.69
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	4	4.69
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	4	4.69
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	4	4.69
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	4	4.69
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	5	4.64
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	5	4.64
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	5	4.64
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	5	4.64
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	5	4.64
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	5	4.64
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	5	4.64
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	5	4.64
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	5	4.64
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	12	4.63
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	12	4.63
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	12	4.63
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	6	4.63
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	6	4.63
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	6	4.63
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	6	4.63
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	6	4.63
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	6	4.63
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	6	4.63
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	6	4.63
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	6	4.63
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	2	4.62
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	2	4.62
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	2	4.62
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	2	4.62
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	2	4.62
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	2	4.62
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	2	4.62
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	2	4.62
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	2	4.62
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	10	4.6
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	10	4.6
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	10	4.6
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	10	4.6
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	10	4.6
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	10	4.6
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	10	4.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	10	4.6
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	10	4.6
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	3	4.59
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	3	4.59
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	3	4.59
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	3	4.59
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	3	4.59
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	3	4.59
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	3	4.59
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	3	4.59
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	3	4.59
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	10	4.58
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	10	4.58
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	10	4.58
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	12	4.58
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	12	4.58
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	12	4.58
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	12	4.58
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	12	4.58
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	12	4.58
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	12	4.58
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	12	4.58
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	12	4.58
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	3	4.57
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	3	4.57
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	3	4.57
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	5	4.57
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	5	4.57
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	5	4.57
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	5	4.57
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	5	4.57
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	5	4.57
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	5	4.57
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	5	4.57
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	5	4.57
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	15	4.54
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	15	4.54
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	15	4.54
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	15	4.54
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	15	4.54
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	15	4.54
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	15	4.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	15	4.54
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	15	4.54
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	10	4.51
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	10	4.51
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	10	4.51
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	10	4.51
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	10	4.51
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	10	4.51
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	10	4.51
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	10	4.51
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	10	4.51
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	8	4.47
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	8	4.47
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	8	4.47
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	8	4.47
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	8	4.47
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	8	4.47
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	8	4.47
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	8	4.47
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	8	4.47
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD21	1	4.46
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD22	1	4.46
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD23	1	4.46
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD21	1	4.46
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD22	1	4.46
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD23	1	4.46
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD21	1	4.46
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD22	1	4.46
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD23	1	4.46
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	3	4.46
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	3	4.46
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	3	4.46
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	3	4.46
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	3	4.46
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	3	4.46
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	3	4.46
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	3	4.46
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	3	4.46
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD21	11	4.44
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD22	11	4.44
(1,376)	1:195:A:VAL:HG21	1:275:A:LEU:HD23	11	4.44
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD21	11	4.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD22	11	4.44
(1,376)	1:195:A:VAL:HG22	1:275:A:LEU:HD23	11	4.44
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD21	11	4.44
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD22	11	4.44
(1,376)	1:195:A:VAL:HG23	1:275:A:LEU:HD23	11	4.44
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	2	4.42
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	2	4.42
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	2	4.42
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	2	4.42
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	2	4.42
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	2	4.42
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	2	4.42
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	2	4.42
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	2	4.42
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	9	4.36
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	9	4.36
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	9	4.36
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	9	4.36
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	9	4.36
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	9	4.36
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	9	4.36
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	9	4.36
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	9	4.36
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	12	4.34
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	12	4.34
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	12	4.34
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	12	4.34
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	12	4.34
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	12	4.34
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	12	4.34
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	12	4.34
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	12	4.34
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	12	4.33
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	12	4.33
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	12	4.33
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	12	4.33
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	12	4.33
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	12	4.33
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	12	4.33
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	12	4.33
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	12	4.33
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	5	4.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	5	4.29
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	5	4.29
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	5	4.29
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	5	4.29
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	5	4.29
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	5	4.29
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	5	4.29
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	5	4.29
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	13	4.28
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	13	4.28
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	13	4.28
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	13	4.28
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	13	4.28
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	13	4.28
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	13	4.28
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	13	4.28
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	13	4.28
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	4	4.24
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	4	4.24
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	4	4.24
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	4	4.24
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	4	4.24
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	4	4.24
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	4	4.24
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	4	4.24
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	4	4.24
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	15	4.23
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	15	4.23
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	15	4.23
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD21	10	4.23
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD22	10	4.23
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD23	10	4.23
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD21	10	4.23
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD22	10	4.23
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD23	10	4.23
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD21	10	4.23
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD22	10	4.23
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD23	10	4.23
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	2	4.19
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	2	4.19
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	2	4.19
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	5	4.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	5	4.18
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	5	4.18
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	5	4.18
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	5	4.18
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	5	4.18
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	5	4.18
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	5	4.18
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	5	4.18
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	6	4.02
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	6	4.02
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	6	4.02
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	11	4.01
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	11	4.01
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	11	4.01
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	11	4.01
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	11	4.01
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	11	4.01
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	11	4.01
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	11	4.01
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	11	4.01
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	9	4.0
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	9	4.0
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	9	4.0
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	9	4.0
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	9	4.0
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	9	4.0
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	9	4.0
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	9	4.0
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	9	4.0
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	6	3.97
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	6	3.97
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	6	3.97
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	6	3.97
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	6	3.97
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	6	3.97
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	6	3.97
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	6	3.97
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	6	3.97
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	2	3.9
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	2	3.9
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	2	3.9
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	11	3.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	11	3.9
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	11	3.9
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	11	3.88
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	11	3.88
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	11	3.88
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	11	3.88
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	11	3.88
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	11	3.88
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	11	3.88
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	11	3.88
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	11	3.88
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	14	3.87
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	14	3.87
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	14	3.87
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	14	3.87
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	14	3.87
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	14	3.87
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	14	3.87
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	14	3.87
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	14	3.87
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG11	4	3.83
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG12	4	3.83
(1,339)	1:179:A:VAL:HG11	1:126:A:VAL:HG13	4	3.83
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG11	4	3.83
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG12	4	3.83
(1,339)	1:179:A:VAL:HG12	1:126:A:VAL:HG13	4	3.83
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG11	4	3.83
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG12	4	3.83
(1,339)	1:179:A:VAL:HG13	1:126:A:VAL:HG13	4	3.83
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	4	3.81
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	4	3.81
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	4	3.81
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	13	3.8
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	13	3.8
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	13	3.8
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	13	3.8
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	13	3.8
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	13	3.8
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	13	3.8
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	13	3.8
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	13	3.8
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	13	3.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	13	3.77
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	13	3.77
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	13	3.77
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	13	3.77
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	13	3.77
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	13	3.77
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	13	3.77
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	13	3.77
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	1	3.77
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	1	3.77
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	1	3.77
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	1	3.77
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	1	3.77
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	1	3.77
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	1	3.77
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	1	3.77
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	1	3.77
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD11	10	3.75
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD12	10	3.75
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD13	10	3.75
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD11	10	3.75
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD12	10	3.75
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD13	10	3.75
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD11	10	3.75
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD12	10	3.75
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD13	10	3.75
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	6	3.73
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	6	3.73
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	6	3.73
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	6	3.73
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	6	3.73
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	6	3.73
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	6	3.73
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	6	3.73
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	6	3.73
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD21	6	3.72
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD22	6	3.72
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD23	6	3.72
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD21	6	3.72
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD22	6	3.72
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD23	6	3.72
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD21	6	3.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD22	6	3.72
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD23	6	3.72
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	15	3.71
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	15	3.71
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	15	3.71
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	15	3.71
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	15	3.71
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	15	3.71
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	15	3.71
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	15	3.71
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	15	3.71
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD21	10	3.7
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD22	10	3.7
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD23	10	3.7
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD21	10	3.7
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD22	10	3.7
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD23	10	3.7
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD21	10	3.7
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD22	10	3.7
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD23	10	3.7
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	9	3.7
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	9	3.7
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	9	3.7
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	9	3.7
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	9	3.7
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	9	3.7
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	9	3.7
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	9	3.7
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	9	3.7
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	4	3.69
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	4	3.69
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	4	3.69
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	4	3.67
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	4	3.67
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	4	3.67
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	4	3.67
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	4	3.67
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	4	3.67
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	4	3.67
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	4	3.67
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	4	3.67
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	12	3.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	12	3.64
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	12	3.64
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	12	3.64
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	12	3.64
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	12	3.64
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	12	3.64
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	12	3.64
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	12	3.64
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	14	3.64
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	14	3.64
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	14	3.64
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	14	3.64
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	14	3.64
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	14	3.64
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	14	3.64
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	14	3.64
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	14	3.64
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	5	3.6
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	5	3.6
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	5	3.6
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD11	11	3.59
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD12	11	3.59
(1,375)	1:195:A:VAL:HG21	1:275:A:LEU:HD13	11	3.59
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD11	11	3.59
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD12	11	3.59
(1,375)	1:195:A:VAL:HG22	1:275:A:LEU:HD13	11	3.59
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD11	11	3.59
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD12	11	3.59
(1,375)	1:195:A:VAL:HG23	1:275:A:LEU:HD13	11	3.59
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	3	3.59
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	3	3.59
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	3	3.59
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	3	3.59
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	3	3.59
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	3	3.59
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	3	3.59
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	3	3.59
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	3	3.59
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	7	3.57
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	7	3.57
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	7	3.57
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	7	3.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	7	3.57
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	7	3.57
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	7	3.57
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	7	3.57
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	7	3.57
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD21	4	3.55
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD22	4	3.55
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD23	4	3.55
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD21	4	3.55
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD22	4	3.55
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD23	4	3.55
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD21	4	3.55
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD22	4	3.55
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD23	4	3.55
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	3	3.46
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	3	3.46
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	3	3.46
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	3	3.46
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	3	3.46
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	3	3.46
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	3	3.46
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	3	3.46
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	3	3.46
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	8	3.45
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	8	3.45
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	8	3.45
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	8	3.45
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	8	3.45
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	8	3.45
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	8	3.45
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	8	3.45
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	8	3.45
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	12	3.44
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	12	3.44
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	12	3.44
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	12	3.43
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	12	3.43
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	12	3.43
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	8	3.43
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	8	3.43
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	8	3.43
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	8	3.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	8	3.43
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	8	3.43
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	8	3.43
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	8	3.43
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	8	3.43
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	9	3.41
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	9	3.41
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	9	3.41
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD21	12	3.41
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD22	12	3.41
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD23	12	3.41
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD21	12	3.41
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD22	12	3.41
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD23	12	3.41
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD21	12	3.41
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD22	12	3.41
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD23	12	3.41
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	15	3.39
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	15	3.39
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	15	3.39
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	8	3.39
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	8	3.39
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	8	3.39
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	8	3.39
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	8	3.39
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	8	3.39
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	8	3.39
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	8	3.39
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	8	3.39
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	5	3.38
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	5	3.38
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	5	3.38
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	6	3.37
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	6	3.37
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	6	3.37
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	6	3.37
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	6	3.37
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	6	3.37
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	6	3.37
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	6	3.37
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	6	3.37
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	14	3.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	14	3.33
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	14	3.33
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	15	3.33
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	15	3.33
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	15	3.33
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	8	3.32
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	8	3.32
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	8	3.32
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	8	3.32
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	8	3.32
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	8	3.32
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	8	3.32
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	8	3.32
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	8	3.32
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	8	3.3
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	8	3.3
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	8	3.3
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	8	3.3
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	8	3.3
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	8	3.3
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	8	3.3
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	8	3.3
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	8	3.3
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	10	3.26
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	10	3.26
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	10	3.26
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	10	3.26
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	10	3.26
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	10	3.26
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	10	3.26
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	10	3.26
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	10	3.26
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD11	4	3.25
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD12	4	3.25
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD13	4	3.25
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD11	4	3.25
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD12	4	3.25
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD13	4	3.25
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD11	4	3.25
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD12	4	3.25
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD13	4	3.25
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	14	3.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	14	3.24
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	14	3.24
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	9	3.24
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	9	3.24
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	9	3.24
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	9	3.24
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	9	3.24
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	9	3.24
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	9	3.24
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	9	3.24
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	9	3.24
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	5	3.23
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	5	3.23
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	5	3.23
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	5	3.23
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	5	3.23
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	5	3.23
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	5	3.23
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	5	3.23
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	5	3.23
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	10	3.23
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	10	3.23
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	10	3.23
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	10	3.23
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	10	3.23
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	10	3.23
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	10	3.23
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	10	3.23
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	10	3.23
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	11	3.22
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	11	3.22
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	11	3.22
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	11	3.22
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	11	3.22
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	11	3.22
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	11	3.22
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	11	3.22
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	11	3.22
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	6	3.21
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	6	3.21
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	6	3.21
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	4	3.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	4	3.19
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	4	3.19
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	15	3.19
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	15	3.19
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	15	3.19
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	15	3.19
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	15	3.19
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	15	3.19
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	15	3.19
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	15	3.19
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	15	3.19
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	13	3.18
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	13	3.18
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	13	3.18
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	13	3.18
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	13	3.18
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	13	3.18
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	13	3.18
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	13	3.18
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	13	3.18
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD21	13	3.16
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD22	13	3.16
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD23	13	3.16
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD21	13	3.16
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD22	13	3.16
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD23	13	3.16
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD21	13	3.16
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD22	13	3.16
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD23	13	3.16
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	1	3.15
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	1	3.15
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	1	3.15
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	1	3.15
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	1	3.15
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	1	3.15
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	1	3.15
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	1	3.15
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	1	3.15
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	4	3.14
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	4	3.14
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	4	3.14
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	4	3.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	4	3.14
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	4	3.14
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	4	3.14
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	4	3.14
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	4	3.14
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	11	3.12
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	11	3.12
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	11	3.12
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	12	3.12
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	12	3.12
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	12	3.12
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	12	3.12
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	12	3.12
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	12	3.12
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	12	3.12
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	12	3.12
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	12	3.12
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	8	3.09
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	8	3.09
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	8	3.09
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	7	3.07
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	7	3.07
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	7	3.07
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	14	3.06
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	14	3.06
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	14	3.06
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	14	3.06
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	14	3.06
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	14	3.06
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	14	3.06
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	14	3.06
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	14	3.06
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	15	3.06
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	15	3.06
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	15	3.06
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	15	3.06
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	15	3.06
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	15	3.06
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	15	3.06
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	15	3.06
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	15	3.06
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	7	3.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	7	3.05
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	7	3.05
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	12	3.04
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	12	3.04
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	12	3.04
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	12	3.04
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	12	3.04
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	12	3.04
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	12	3.04
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	12	3.04
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	12	3.04
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	2	3.04
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	2	3.04
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	2	3.04
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	2	3.04
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	2	3.04
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	2	3.04
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	2	3.04
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	2	3.04
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	2	3.04
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	13	3.03
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	13	3.03
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	13	3.03
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	6	3.0
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	6	3.0
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	6	3.0
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	6	3.0
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	6	3.0
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	6	3.0
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	6	3.0
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	6	3.0
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	6	3.0
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	4	2.98
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	4	2.98
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	4	2.98
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	4	2.98
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	4	2.98
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	4	2.98
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	4	2.98
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	4	2.98
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	4	2.98
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	15	2.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	15	2.98
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	15	2.98
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	15	2.98
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	15	2.98
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	15	2.98
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	15	2.98
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	15	2.98
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	15	2.98
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	7	2.97
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	7	2.97
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	7	2.97
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	7	2.97
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	7	2.97
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	7	2.97
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	7	2.97
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	7	2.97
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	7	2.97
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	7	2.97
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	7	2.97
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	7	2.97
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD21	3	2.96
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD22	3	2.96
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD23	3	2.96
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD21	3	2.96
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD22	3	2.96
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD23	3	2.96
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD21	3	2.96
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD22	3	2.96
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD23	3	2.96
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	5	2.95
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	5	2.95
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	5	2.95
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	5	2.95
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	5	2.95
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	5	2.95
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	5	2.95
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	5	2.95
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	5	2.95
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	13	2.9
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	13	2.9
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	13	2.9
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	13	2.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	13	2.9
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	13	2.9
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	13	2.9
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	13	2.9
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	13	2.9
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	4	2.89
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	4	2.89
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	4	2.89
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	4	2.89
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	4	2.89
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	4	2.89
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	4	2.89
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	4	2.89
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	4	2.89
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	11	2.89
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	11	2.89
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	11	2.89
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	11	2.89
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	11	2.89
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	11	2.89
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	11	2.89
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	11	2.89
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	11	2.89
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	13	2.89
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	13	2.89
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	13	2.89
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	3	2.88
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	3	2.88
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	3	2.88
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	3	2.88
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	3	2.88
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	3	2.88
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	3	2.88
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	3	2.88
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	3	2.88
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	5	2.85
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	5	2.85
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	5	2.85
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	5	2.85
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	5	2.85
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	5	2.85
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	5	2.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	5	2.85
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	5	2.85
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	11	2.85
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	11	2.85
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	11	2.85
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	11	2.85
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	11	2.85
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	11	2.85
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	11	2.85
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	11	2.85
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	11	2.85
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	3	2.84
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	3	2.84
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	3	2.84
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	3	2.84
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	3	2.84
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	3	2.84
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	3	2.84
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	3	2.84
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	3	2.84
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD11	15	2.84
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD12	15	2.84
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD13	15	2.84
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD11	15	2.84
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD12	15	2.84
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD13	15	2.84
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD11	15	2.84
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD12	15	2.84
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD13	15	2.84
(1,352)	1:167:A:LEU:HD21	1:202:A:GLN:H	6	2.84
(1,352)	1:167:A:LEU:HD22	1:202:A:GLN:H	6	2.84
(1,352)	1:167:A:LEU:HD23	1:202:A:GLN:H	6	2.84
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	11	2.83
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	11	2.83
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	11	2.83
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	11	2.83
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	11	2.83
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	11	2.83
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	11	2.83
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	11	2.83
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	11	2.83
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	2	2.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	2	2.82
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	2	2.82
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	2	2.82
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	2	2.82
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	2	2.82
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	2	2.82
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	2	2.82
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	2	2.82
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	5	2.78
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	5	2.78
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	5	2.78
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	5	2.78
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	5	2.78
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	5	2.78
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	5	2.78
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	5	2.78
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	5	2.78
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	13	2.73
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	13	2.73
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	13	2.73
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	12	2.72
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	12	2.72
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	12	2.72
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB1	12	2.72
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB2	12	2.72
(1,368)	1:189:A:LEU:HD11	1:231:A:ALA:HB3	12	2.72
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB1	12	2.72
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB2	12	2.72
(1,368)	1:189:A:LEU:HD12	1:231:A:ALA:HB3	12	2.72
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB1	12	2.72
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB2	12	2.72
(1,368)	1:189:A:LEU:HD13	1:231:A:ALA:HB3	12	2.72
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD11	12	2.72
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD12	12	2.72
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD13	12	2.72
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD11	12	2.72
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD12	12	2.72
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD13	12	2.72
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD11	12	2.72
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD12	12	2.72
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD13	12	2.72
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	12	2.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	12	2.71
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	12	2.71
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	1	2.67
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	1	2.67
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	1	2.67
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	1	2.67
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	1	2.67
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	1	2.67
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	1	2.67
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	1	2.67
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	1	2.67
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	2	2.67
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	2	2.67
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	2	2.67
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	2	2.67
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	2	2.67
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	2	2.67
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	2	2.67
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	2	2.67
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	2	2.67
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	1	2.65
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	1	2.65
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	1	2.65
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	7	2.65
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	7	2.65
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	7	2.65
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	9	2.64
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	9	2.64
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	9	2.64
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	9	2.64
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	9	2.64
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	9	2.64
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	9	2.64
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	9	2.64
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	9	2.64
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	6	2.64
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	6	2.64
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	6	2.64
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	6	2.64
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	6	2.64
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	6	2.64
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	6	2.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	6	2.64
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	6	2.64
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG21	15	2.63
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG22	15	2.63
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG23	15	2.63
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG21	15	2.63
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG22	15	2.63
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG23	15	2.63
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG21	15	2.63
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG22	15	2.63
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG23	15	2.63
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	9	2.63
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	9	2.63
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	9	2.63
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	14	2.63
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	14	2.63
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	14	2.63
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	15	2.63
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	15	2.63
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	15	2.63
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	15	2.63
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	15	2.63
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	15	2.63
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	15	2.63
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	15	2.63
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	15	2.63
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	4	2.62
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	4	2.62
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	4	2.62
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	4	2.62
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	4	2.62
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	4	2.62
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	4	2.62
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	4	2.62
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	4	2.62
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	10	2.61
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	10	2.61
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	10	2.61
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	13	2.6
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	13	2.6
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	13	2.6
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	13	2.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	13	2.59
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	13	2.59
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	7	2.57
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	7	2.57
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	7	2.57
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	7	2.57
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	7	2.57
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	7	2.57
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	7	2.57
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	7	2.57
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	7	2.57
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	4	2.55
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	4	2.55
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	4	2.55
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	4	2.55
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	4	2.55
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	4	2.55
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	4	2.55
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	4	2.55
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	4	2.55
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	2	2.54
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	2	2.54
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	2	2.54
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	2	2.54
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	2	2.54
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	2	2.54
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	2	2.54
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	2	2.54
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	2	2.54
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	12	2.53
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	12	2.53
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	12	2.53
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	12	2.53
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	12	2.53
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	12	2.53
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	12	2.53
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	12	2.53
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	12	2.53
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG11	6	2.53
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG12	6	2.53
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG13	6	2.53
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG11	6	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG12	6	2.53
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG13	6	2.53
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG11	6	2.53
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG12	6	2.53
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG13	6	2.53
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	6	2.49
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	6	2.49
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	6	2.49
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	6	2.49
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	6	2.49
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	6	2.49
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	6	2.49
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	6	2.49
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	6	2.49
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD11	7	2.49
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD12	7	2.49
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD13	7	2.49
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD11	7	2.49
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD12	7	2.49
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD13	7	2.49
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD11	7	2.49
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD12	7	2.49
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD13	7	2.49
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	6	2.48
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	6	2.48
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	6	2.48
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	10	2.48
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	10	2.48
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	10	2.48
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	1	2.47
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	1	2.47
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	1	2.47
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	10	2.46
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	10	2.46
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	10	2.46
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	10	2.46
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	10	2.46
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	10	2.46
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	10	2.46
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	10	2.46
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	10	2.46
(1,352)	1:167:A:LEU:HD21	1:202:A:GLN:H	4	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:167:A:LEU:HD22	1:202:A:GLN:H	4	2.46
(1,352)	1:167:A:LEU:HD23	1:202:A:GLN:H	4	2.46
(1,345)	1:163:A:LEU:HD11	1:157:A:LEU:H	6	2.45
(1,345)	1:163:A:LEU:HD12	1:157:A:LEU:H	6	2.45
(1,345)	1:163:A:LEU:HD13	1:157:A:LEU:H	6	2.45
(1,358)	1:176:A:LEU:HD11	1:196:A:TYR:H	7	2.44
(1,358)	1:176:A:LEU:HD12	1:196:A:TYR:H	7	2.44
(1,358)	1:176:A:LEU:HD13	1:196:A:TYR:H	7	2.44
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	8	2.44
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	8	2.44
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	8	2.44
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	8	2.44
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	8	2.44
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	8	2.44
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	8	2.44
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	8	2.44
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	8	2.44
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	9	2.44
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	9	2.44
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	9	2.44
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	9	2.44
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	9	2.44
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	9	2.44
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	9	2.44
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	9	2.44
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	9	2.44
(1,351)	1:167:A:LEU:HD11	1:124:A:ILE:H	13	2.43
(1,351)	1:167:A:LEU:HD12	1:124:A:ILE:H	13	2.43
(1,351)	1:167:A:LEU:HD13	1:124:A:ILE:H	13	2.43
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	14	2.41
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	14	2.41
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	14	2.41
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	14	2.41
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	14	2.41
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	14	2.41
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	14	2.41
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	14	2.41
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	14	2.41
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	12	2.4
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	12	2.4
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	12	2.4
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	12	2.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	12	2.4
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	12	2.4
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	12	2.4
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	12	2.4
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	12	2.4
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	7	2.4
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	7	2.4
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	7	2.4
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	7	2.4
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	7	2.4
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	7	2.4
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	7	2.4
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	7	2.4
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	7	2.4
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	5	2.39
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	5	2.39
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	5	2.39
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	5	2.39
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	5	2.39
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	5	2.39
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	5	2.39
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	5	2.39
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	5	2.39
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	3	2.38
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	3	2.38
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	3	2.38
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	8	2.38
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	8	2.38
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	8	2.38
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	8	2.38
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	8	2.38
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	8	2.38
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	8	2.38
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	8	2.38
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	8	2.38
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	15	2.37
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	15	2.37
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	15	2.37
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	15	2.37
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	15	2.37
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	15	2.37
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	15	2.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	15	2.37
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	15	2.37
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD21	4	2.36
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD22	4	2.36
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD23	4	2.36
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD21	4	2.36
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD22	4	2.36
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD23	4	2.36
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD21	4	2.36
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD22	4	2.36
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD23	4	2.36
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD11	6	2.36
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD12	6	2.36
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD13	6	2.36
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD11	6	2.36
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD12	6	2.36
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD13	6	2.36
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD11	6	2.36
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD12	6	2.36
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD13	6	2.36
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	10	2.35
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	10	2.35
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	10	2.35
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	10	2.35
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	10	2.35
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	10	2.35
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	10	2.35
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	10	2.35
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	10	2.35
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	10	2.35
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	10	2.35
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	10	2.35
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	1	2.32
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	1	2.32
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	1	2.32
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	1	2.32
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	1	2.32
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	1	2.32
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	1	2.32
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	1	2.32
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	1	2.32
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	1	2.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	1	2.29
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	1	2.29
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	1	2.29
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	1	2.29
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	1	2.29
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	1	2.29
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	1	2.29
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	1	2.29
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	15	2.27
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	15	2.27
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	15	2.27
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	15	2.27
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	15	2.27
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	15	2.27
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	15	2.27
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	15	2.27
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	15	2.27
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	15	2.26
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	15	2.26
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	15	2.26
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	15	2.26
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	15	2.26
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	15	2.26
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	15	2.26
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	15	2.26
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	15	2.26
(1,352)	1:167:A:LEU:HD21	1:202:A:GLN:H	14	2.26
(1,352)	1:167:A:LEU:HD22	1:202:A:GLN:H	14	2.26
(1,352)	1:167:A:LEU:HD23	1:202:A:GLN:H	14	2.26
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	9	2.26
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	9	2.26
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	9	2.26
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	9	2.26
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	9	2.26
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	9	2.26
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	9	2.26
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	9	2.26
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	9	2.26
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	1	2.25
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	1	2.25
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	1	2.25
(1,351)	1:167:A:LEU:HD11	1:124:A:ILE:H	12	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:167:A:LEU:HD12	1:124:A:ILE:H	12	2.25
(1,351)	1:167:A:LEU:HD13	1:124:A:ILE:H	12	2.25
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	14	2.23
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	14	2.23
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	14	2.23
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	14	2.23
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	14	2.23
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	14	2.23
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	14	2.23
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	14	2.23
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	14	2.23
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG21	6	2.21
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG22	6	2.21
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG23	6	2.21
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG21	6	2.21
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG22	6	2.21
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG23	6	2.21
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG21	6	2.21
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG22	6	2.21
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG23	6	2.21
(1,352)	1:167:A:LEU:HD21	1:202:A:GLN:H	3	2.2
(1,352)	1:167:A:LEU:HD22	1:202:A:GLN:H	3	2.2
(1,352)	1:167:A:LEU:HD23	1:202:A:GLN:H	3	2.2
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD11	1	2.2
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD12	1	2.2
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD13	1	2.2
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD11	1	2.2
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD12	1	2.2
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD13	1	2.2
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD11	1	2.2
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD12	1	2.2
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD13	1	2.2
(1,382)	1:205:A:ILE:HG21	1:216:A:THR:H	15	2.19
(1,382)	1:205:A:ILE:HG22	1:216:A:THR:H	15	2.19
(1,382)	1:205:A:ILE:HG23	1:216:A:THR:H	15	2.19
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG21	8	2.18
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG22	8	2.18
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG23	8	2.18
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG21	8	2.18
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG22	8	2.18
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG23	8	2.18
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG21	8	2.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG22	8	2.18
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG23	8	2.18
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	14	2.17
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	14	2.17
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	14	2.17
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD11	1	2.17
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD12	1	2.17
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD13	1	2.17
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD11	1	2.17
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD12	1	2.17
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD13	1	2.17
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD11	1	2.17
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD12	1	2.17
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD13	1	2.17
(1,319)	1:89:A:LEU:HD11	1:95:A:ASN:H	4	2.17
(1,319)	1:89:A:LEU:HD12	1:95:A:ASN:H	4	2.17
(1,319)	1:89:A:LEU:HD13	1:95:A:ASN:H	4	2.17
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	8	2.16
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	8	2.16
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	8	2.16
(1,358)	1:176:A:LEU:HD11	1:196:A:TYR:H	14	2.16
(1,358)	1:176:A:LEU:HD12	1:196:A:TYR:H	14	2.16
(1,358)	1:176:A:LEU:HD13	1:196:A:TYR:H	14	2.16
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	14	2.15
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	14	2.15
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	14	2.15
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	14	2.15
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	14	2.15
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	14	2.15
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	14	2.15
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	14	2.15
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	14	2.15
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	2	2.15
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	2	2.15
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	2	2.15
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	4	2.14
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	4	2.14
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	4	2.14
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	4	2.14
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	4	2.14
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	4	2.14
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	4	2.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	4	2.14
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	4	2.14
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD11	9	2.12
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD12	9	2.12
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD13	9	2.12
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD11	9	2.12
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD12	9	2.12
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD13	9	2.12
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD11	9	2.12
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD12	9	2.12
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD13	9	2.12
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	13	2.1
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	13	2.1
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	13	2.1
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	11	2.09
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	11	2.09
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	11	2.09
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	11	2.09
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	11	2.09
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	11	2.09
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	11	2.09
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	11	2.09
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	11	2.09
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	6	2.08
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	6	2.08
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	6	2.08
(1,345)	1:163:A:LEU:HD11	1:157:A:LEU:H	9	2.08
(1,345)	1:163:A:LEU:HD12	1:157:A:LEU:H	9	2.08
(1,345)	1:163:A:LEU:HD13	1:157:A:LEU:H	9	2.08
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	14	2.08
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	14	2.08
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	14	2.08
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	14	2.08
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	14	2.08
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	14	2.08
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	14	2.08
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	14	2.08
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	14	2.08
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG21	15	2.07
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG22	15	2.07
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG23	15	2.07
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG21	15	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG22	15	2.07
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG23	15	2.07
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG21	15	2.07
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG22	15	2.07
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG23	15	2.07
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	11	2.06
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	11	2.06
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	11	2.06
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	11	2.06
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	11	2.06
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	11	2.06
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	11	2.06
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	11	2.06
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	11	2.06
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	1	2.06
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	1	2.06
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	1	2.06
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	1	2.06
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	1	2.06
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	1	2.06
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	1	2.06
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	1	2.06
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	1	2.06
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	2	2.05
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	2	2.05
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	2	2.05
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	2	2.05
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	2	2.05
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	2	2.05
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	2	2.05
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	2	2.05
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	2	2.05
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD21	12	2.05
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD22	12	2.05
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD23	12	2.05
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD21	12	2.05
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD22	12	2.05
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD23	12	2.05
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD21	12	2.05
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD22	12	2.05
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD23	12	2.05
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	6	2.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	6	2.05
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	6	2.05
(1,395)	1:237:A:ILE:HD11	1:228:A:LEU:H	12	2.04
(1,395)	1:237:A:ILE:HD12	1:228:A:LEU:H	12	2.04
(1,395)	1:237:A:ILE:HD13	1:228:A:LEU:H	12	2.04
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	11	2.04
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	11	2.04
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	11	2.04
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	11	2.04
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	11	2.04
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	11	2.04
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	11	2.04
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	11	2.04
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	11	2.04
(1,395)	1:237:A:ILE:HD11	1:228:A:LEU:H	13	2.03
(1,395)	1:237:A:ILE:HD12	1:228:A:LEU:H	13	2.03
(1,395)	1:237:A:ILE:HD13	1:228:A:LEU:H	13	2.03
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	2	2.03
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	2	2.03
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	2	2.03
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	2	2.03
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	2	2.03
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	2	2.03
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	2	2.03
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	2	2.03
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	2	2.03
(1,363)	1:179:A:VAL:HG11	1:98:A:GLN:H	1	2.03
(1,363)	1:179:A:VAL:HG12	1:98:A:GLN:H	1	2.03
(1,363)	1:179:A:VAL:HG13	1:98:A:GLN:H	1	2.03
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	11	2.03
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	11	2.03
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	11	2.03
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	11	2.03
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	11	2.03
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	11	2.03
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	11	2.03
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	11	2.03
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	11	2.03
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	3	2.01
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	3	2.01
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	3	2.01
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD21	7	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD22	7	2.01
(1,366)	1:182:A:ILE:HG21	1:228:A:LEU:HD23	7	2.01
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD21	7	2.01
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD22	7	2.01
(1,366)	1:182:A:ILE:HG22	1:228:A:LEU:HD23	7	2.01
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD21	7	2.01
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD22	7	2.01
(1,366)	1:182:A:ILE:HG23	1:228:A:LEU:HD23	7	2.01
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	15	2.01
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	15	2.01
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	15	2.01
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	15	2.01
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	15	2.01
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	15	2.01
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	15	2.01
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	15	2.01
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	15	2.01
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	9	2.01
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	9	2.01
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	9	2.01
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	9	2.01
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	9	2.01
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	9	2.01
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	9	2.01
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	9	2.01
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	9	2.01
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG21	4	1.99
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG22	4	1.99
(1,326)	1:101:A:LEU:HD21	1:179:A:VAL:HG23	4	1.99
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG21	4	1.99
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG22	4	1.99
(1,326)	1:101:A:LEU:HD22	1:179:A:VAL:HG23	4	1.99
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG21	4	1.99
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG22	4	1.99
(1,326)	1:101:A:LEU:HD23	1:179:A:VAL:HG23	4	1.99
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	14	1.98
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	14	1.98
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	14	1.98
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	14	1.98
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	14	1.98
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	14	1.98
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	14	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	14	1.98
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	14	1.98
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	7	1.98
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	7	1.98
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	7	1.98
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	7	1.98
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	7	1.98
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	7	1.98
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	7	1.98
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	7	1.98
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	7	1.98
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	2	1.98
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	2	1.98
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	2	1.98
(1,351)	1:167:A:LEU:HD11	1:124:A:ILE:H	10	1.98
(1,351)	1:167:A:LEU:HD12	1:124:A:ILE:H	10	1.98
(1,351)	1:167:A:LEU:HD13	1:124:A:ILE:H	10	1.98
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD21	3	1.96
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD22	3	1.96
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD23	3	1.96
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD21	3	1.96
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD22	3	1.96
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD23	3	1.96
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD21	3	1.96
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD22	3	1.96
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD23	3	1.96
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	12	1.96
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	12	1.96
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	12	1.96
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	12	1.96
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	12	1.96
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	12	1.96
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	12	1.96
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	12	1.96
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	12	1.96
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	11	1.95
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	11	1.95
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	11	1.95
(1,351)	1:167:A:LEU:HD11	1:124:A:ILE:H	5	1.91
(1,351)	1:167:A:LEU:HD12	1:124:A:ILE:H	5	1.91
(1,351)	1:167:A:LEU:HD13	1:124:A:ILE:H	5	1.91
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD21	6	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD22	6	1.9
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD23	6	1.9
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD21	6	1.9
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD22	6	1.9
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD23	6	1.9
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD21	6	1.9
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD22	6	1.9
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD23	6	1.9
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD11	4	1.86
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD12	4	1.86
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD13	4	1.86
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD11	4	1.86
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD12	4	1.86
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD13	4	1.86
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD11	4	1.86
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD12	4	1.86
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD13	4	1.86
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	9	1.86
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	9	1.86
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	9	1.86
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	9	1.86
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	9	1.86
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	9	1.86
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	9	1.86
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	9	1.86
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	9	1.86
(1,385)	1:207:A:VAL:HG21	1:162:A:THR:H	2	1.83
(1,385)	1:207:A:VAL:HG22	1:162:A:THR:H	2	1.83
(1,385)	1:207:A:VAL:HG23	1:162:A:THR:H	2	1.83
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	8	1.82
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	8	1.82
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	8	1.82
(1,319)	1:89:A:LEU:HD11	1:95:A:ASN:H	11	1.8
(1,319)	1:89:A:LEU:HD12	1:95:A:ASN:H	11	1.8
(1,319)	1:89:A:LEU:HD13	1:95:A:ASN:H	11	1.8
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	11	1.79
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	11	1.79
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	11	1.79
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	11	1.79
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	11	1.79
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	11	1.79
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	11	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	11	1.79
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	11	1.79
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	3	1.78
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	3	1.78
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	3	1.78
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	3	1.78
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	3	1.78
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	3	1.78
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	3	1.78
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	3	1.78
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	3	1.78
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	15	1.78
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	15	1.78
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	15	1.78
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	15	1.78
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	15	1.78
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	15	1.78
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	15	1.78
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	15	1.78
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	15	1.78
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	3	1.78
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	3	1.78
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	3	1.78
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	3	1.78
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	3	1.78
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	3	1.78
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	3	1.78
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	3	1.78
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	3	1.78
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG21	10	1.78
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG22	10	1.78
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG23	10	1.78
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG21	10	1.78
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG22	10	1.78
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG23	10	1.78
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG21	10	1.78
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG22	10	1.78
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG23	10	1.78
(1,340)	1:157:A:LEU:HD11	1:162:A:THR:HG21	5	1.76
(1,340)	1:157:A:LEU:HD11	1:162:A:THR:HG22	5	1.76
(1,340)	1:157:A:LEU:HD11	1:162:A:THR:HG23	5	1.76
(1,340)	1:157:A:LEU:HD12	1:162:A:THR:HG21	5	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:157:A:LEU:HD12	1:162:A:THR:HG22	5	1.76
(1,340)	1:157:A:LEU:HD12	1:162:A:THR:HG23	5	1.76
(1,340)	1:157:A:LEU:HD13	1:162:A:THR:HG21	5	1.76
(1,340)	1:157:A:LEU:HD13	1:162:A:THR:HG22	5	1.76
(1,340)	1:157:A:LEU:HD13	1:162:A:THR:HG23	5	1.76
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	6	1.75
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	6	1.75
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	6	1.75
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	6	1.75
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	6	1.75
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	6	1.75
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	6	1.75
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	6	1.75
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	6	1.75
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG21	6	1.74
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG22	6	1.74
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG23	6	1.74
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG21	6	1.74
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG22	6	1.74
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG23	6	1.74
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG21	6	1.74
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG22	6	1.74
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG23	6	1.74
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	2	1.73
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	2	1.73
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	2	1.73
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	2	1.73
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	2	1.73
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	2	1.73
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	2	1.73
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	2	1.73
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	2	1.73
(1,382)	1:205:A:ILE:HG21	1:216:A:THR:H	8	1.73
(1,382)	1:205:A:ILE:HG22	1:216:A:THR:H	8	1.73
(1,382)	1:205:A:ILE:HG23	1:216:A:THR:H	8	1.73
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	10	1.72
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	10	1.72
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	10	1.72
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD21	5	1.71
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD22	5	1.71
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD23	5	1.71
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD21	5	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD22	5	1.71
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD23	5	1.71
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD21	5	1.71
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD22	5	1.71
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD23	5	1.71
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD11	1	1.7
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD12	1	1.7
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD13	1	1.7
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD11	1	1.7
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD12	1	1.7
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD13	1	1.7
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD11	1	1.7
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD12	1	1.7
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD13	1	1.7
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	7	1.69
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	7	1.69
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	7	1.69
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	7	1.69
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	7	1.69
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	7	1.69
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	7	1.69
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	7	1.69
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	7	1.69
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	14	1.68
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	14	1.68
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	14	1.68
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	14	1.68
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	14	1.68
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	14	1.68
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	14	1.68
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	14	1.68
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	14	1.68
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD11	1	1.67
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD12	1	1.67
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD13	1	1.67
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD11	1	1.67
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD12	1	1.67
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD13	1	1.67
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD11	1	1.67
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD12	1	1.67
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD13	1	1.67
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	2	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	2	1.67
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	2	1.67
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	2	1.67
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	2	1.67
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	2	1.67
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	2	1.67
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	2	1.67
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	2	1.67
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD21	13	1.66
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD22	13	1.66
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD23	13	1.66
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD21	13	1.66
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD22	13	1.66
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD23	13	1.66
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD21	13	1.66
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD22	13	1.66
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD23	13	1.66
(1,351)	1:167:A:LEU:HD11	1:124:A:ILE:H	11	1.66
(1,351)	1:167:A:LEU:HD12	1:124:A:ILE:H	11	1.66
(1,351)	1:167:A:LEU:HD13	1:124:A:ILE:H	11	1.66
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG21	5	1.66
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG22	5	1.66
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG23	5	1.66
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG21	5	1.66
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG22	5	1.66
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG23	5	1.66
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG21	5	1.66
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG22	5	1.66
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG23	5	1.66
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	11	1.65
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	11	1.65
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	11	1.65
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	11	1.65
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	11	1.65
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	11	1.65
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	11	1.65
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	11	1.65
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	11	1.65
(1,382)	1:205:A:ILE:HG21	1:216:A:THR:H	4	1.64
(1,382)	1:205:A:ILE:HG22	1:216:A:THR:H	4	1.64
(1,382)	1:205:A:ILE:HG23	1:216:A:THR:H	4	1.64
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	1	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	1	1.64
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	1	1.64
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	1	1.64
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	1	1.64
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	1	1.64
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	1	1.64
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	1	1.64
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	1	1.64
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	7	1.64
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	7	1.64
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	7	1.64
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	7	1.64
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	7	1.64
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	7	1.64
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	7	1.64
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	7	1.64
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	7	1.64
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	9	1.63
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	9	1.63
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	9	1.63
(1,382)	1:205:A:ILE:HG21	1:216:A:THR:H	10	1.61
(1,382)	1:205:A:ILE:HG22	1:216:A:THR:H	10	1.61
(1,382)	1:205:A:ILE:HG23	1:216:A:THR:H	10	1.61
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD11	14	1.61
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD12	14	1.61
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD13	14	1.61
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD11	14	1.61
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD12	14	1.61
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD13	14	1.61
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD11	14	1.61
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD12	14	1.61
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD13	14	1.61
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	7	1.59
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	7	1.59
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	7	1.59
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	7	1.59
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	7	1.59
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	7	1.59
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	7	1.59
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	7	1.59
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	7	1.59
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG21	13	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG22	13	1.58
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG23	13	1.58
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG21	13	1.58
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG22	13	1.58
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG23	13	1.58
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG21	13	1.58
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG22	13	1.58
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG23	13	1.58
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD21	4	1.57
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD22	4	1.57
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD23	4	1.57
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD21	4	1.57
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD22	4	1.57
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD23	4	1.57
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD21	4	1.57
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD22	4	1.57
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD23	4	1.57
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	3	1.56
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	3	1.56
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	3	1.56
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	3	1.56
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	3	1.56
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	3	1.56
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	3	1.56
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	3	1.56
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	3	1.56
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	6	1.55
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	6	1.55
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	6	1.55
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	6	1.55
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	6	1.55
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	6	1.55
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	6	1.55
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	6	1.55
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	6	1.55
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	5	1.55
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	5	1.55
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	5	1.55
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	15	1.54
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	15	1.54
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	15	1.54
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	15	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	15	1.54
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	15	1.54
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	15	1.54
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	15	1.54
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	15	1.54
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	8	1.53
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	8	1.53
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	8	1.53
(1,358)	1:176:A:LEU:HD11	1:196:A:TYR:H	8	1.52
(1,358)	1:176:A:LEU:HD12	1:196:A:TYR:H	8	1.52
(1,358)	1:176:A:LEU:HD13	1:196:A:TYR:H	8	1.52
(1,382)	1:205:A:ILE:HG21	1:216:A:THR:H	9	1.49
(1,382)	1:205:A:ILE:HG22	1:216:A:THR:H	9	1.49
(1,382)	1:205:A:ILE:HG23	1:216:A:THR:H	9	1.49
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	9	1.49
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	9	1.49
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	9	1.49
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	9	1.49
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	9	1.49
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	9	1.49
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	9	1.49
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	9	1.49
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	9	1.49
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	11	1.49
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	11	1.49
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	11	1.49
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD11	8	1.49
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD12	8	1.49
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD13	8	1.49
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD11	8	1.49
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD12	8	1.49
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD13	8	1.49
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD11	8	1.49
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD12	8	1.49
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD13	8	1.49
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	12	1.48
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	12	1.48
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	12	1.48
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	12	1.48
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	12	1.48
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	12	1.48
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	12	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	12	1.48
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	12	1.48
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD11	15	1.48
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD12	15	1.48
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD13	15	1.48
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD11	15	1.48
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD12	15	1.48
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD13	15	1.48
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD11	15	1.48
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD12	15	1.48
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD13	15	1.48
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD21	15	1.48
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD22	15	1.48
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD23	15	1.48
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD21	15	1.48
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD22	15	1.48
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD23	15	1.48
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD21	15	1.48
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD22	15	1.48
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD23	15	1.48
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	15	1.48
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	15	1.48
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	15	1.48
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	15	1.48
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	15	1.48
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	15	1.48
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	15	1.48
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	15	1.48
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	15	1.48
(1,345)	1:163:A:LEU:HD11	1:157:A:LEU:H	8	1.47
(1,345)	1:163:A:LEU:HD12	1:157:A:LEU:H	8	1.47
(1,345)	1:163:A:LEU:HD13	1:157:A:LEU:H	8	1.47
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	5	1.47
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	5	1.47
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	5	1.47
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	5	1.47
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	5	1.47
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	5	1.47
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	5	1.47
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	5	1.47
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	5	1.47
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	4	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	4	1.46
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	4	1.46
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	4	1.46
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	4	1.46
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	4	1.46
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	4	1.46
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	4	1.46
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	4	1.46
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD11	8	1.45
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD12	8	1.45
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD13	8	1.45
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD11	8	1.45
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD12	8	1.45
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD13	8	1.45
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD11	8	1.45
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD12	8	1.45
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD13	8	1.45
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD21	8	1.45
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD22	8	1.45
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD23	8	1.45
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD21	8	1.45
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD22	8	1.45
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD23	8	1.45
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD21	8	1.45
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD22	8	1.45
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD23	8	1.45
(1,345)	1:163:A:LEU:HD11	1:157:A:LEU:H	4	1.45
(1,345)	1:163:A:LEU:HD12	1:157:A:LEU:H	4	1.45
(1,345)	1:163:A:LEU:HD13	1:157:A:LEU:H	4	1.45
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD11	6	1.44
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD12	6	1.44
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD13	6	1.44
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD11	6	1.44
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD12	6	1.44
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD13	6	1.44
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD11	6	1.44
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD12	6	1.44
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD13	6	1.44
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD21	6	1.44
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD22	6	1.44
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD23	6	1.44
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD21	6	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD22	6	1.44
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD23	6	1.44
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD21	6	1.44
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD22	6	1.44
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD23	6	1.44
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	13	1.44
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	13	1.44
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	13	1.44
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	13	1.44
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	13	1.44
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	13	1.44
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	13	1.44
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	13	1.44
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	13	1.44
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG21	6	1.44
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG22	6	1.44
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG23	6	1.44
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG21	6	1.44
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG22	6	1.44
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG23	6	1.44
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG21	6	1.44
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG22	6	1.44
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG23	6	1.44
(1,396)	1:237:A:ILE:HD11	1:229:A:CYS:H	15	1.43
(1,396)	1:237:A:ILE:HD12	1:229:A:CYS:H	15	1.43
(1,396)	1:237:A:ILE:HD13	1:229:A:CYS:H	15	1.43
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	2	1.43
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	2	1.43
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	2	1.43
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	2	1.43
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	2	1.43
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	2	1.43
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	2	1.43
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	2	1.43
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	2	1.43
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	13	1.42
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	13	1.42
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	13	1.42
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	13	1.42
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	13	1.42
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	13	1.42
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	13	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	13	1.42
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	13	1.42
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	12	1.42
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	12	1.42
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	12	1.42
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	15	1.42
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	15	1.42
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	15	1.42
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG11	7	1.42
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG12	7	1.42
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG13	7	1.42
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG11	7	1.42
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG12	7	1.42
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG13	7	1.42
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG11	7	1.42
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG12	7	1.42
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG13	7	1.42
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	11	1.42
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	11	1.42
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	11	1.42
(1,358)	1:176:A:LEU:HD11	1:196:A:TYR:H	3	1.41
(1,358)	1:176:A:LEU:HD12	1:196:A:TYR:H	3	1.41
(1,358)	1:176:A:LEU:HD13	1:196:A:TYR:H	3	1.41
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	7	1.41
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	7	1.41
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	7	1.41
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD11	12	1.41
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD12	12	1.41
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD13	12	1.41
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD11	12	1.41
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD12	12	1.41
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD13	12	1.41
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD11	12	1.41
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD12	12	1.41
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD13	12	1.41
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD21	12	1.41
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD22	12	1.41
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD23	12	1.41
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD21	12	1.41
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD22	12	1.41
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD23	12	1.41
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD21	12	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD22	12	1.41
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD23	12	1.41
(1,319)	1:89:A:LEU:HD11	1:95:A:ASN:H	3	1.41
(1,319)	1:89:A:LEU:HD12	1:95:A:ASN:H	3	1.41
(1,319)	1:89:A:LEU:HD13	1:95:A:ASN:H	3	1.41
(1,382)	1:205:A:ILE:HG21	1:216:A:THR:H	1	1.4
(1,382)	1:205:A:ILE:HG22	1:216:A:THR:H	1	1.4
(1,382)	1:205:A:ILE:HG23	1:216:A:THR:H	1	1.4
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	2	1.4
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	2	1.4
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	2	1.4
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	2	1.4
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	2	1.4
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	2	1.4
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	2	1.4
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	2	1.4
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	2	1.4
(1,358)	1:176:A:LEU:HD11	1:196:A:TYR:H	11	1.39
(1,358)	1:176:A:LEU:HD12	1:196:A:TYR:H	11	1.39
(1,358)	1:176:A:LEU:HD13	1:196:A:TYR:H	11	1.39
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG21	4	1.38
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG22	4	1.38
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG23	4	1.38
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG21	4	1.38
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG22	4	1.38
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG23	4	1.38
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG21	4	1.38
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG22	4	1.38
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG23	4	1.38
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD11	3	1.37
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD12	3	1.37
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD13	3	1.37
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD11	3	1.37
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD12	3	1.37
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD13	3	1.37
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD11	3	1.37
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD12	3	1.37
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD13	3	1.37
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD21	3	1.37
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD22	3	1.37
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD23	3	1.37
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD21	3	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD22	3	1.37
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD23	3	1.37
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD21	3	1.37
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD22	3	1.37
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD23	3	1.37
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD11	3	1.37
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD12	3	1.37
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD13	3	1.37
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD11	3	1.37
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD12	3	1.37
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD13	3	1.37
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD11	3	1.37
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD12	3	1.37
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD13	3	1.37
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	9	1.37
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	9	1.37
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	9	1.37
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	3	1.37
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	3	1.37
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	3	1.37
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	3	1.37
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	3	1.37
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	3	1.37
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	3	1.37
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	3	1.37
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	3	1.37
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	14	1.37
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	14	1.37
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	14	1.37
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	14	1.37
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	14	1.37
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	14	1.37
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	14	1.37
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	14	1.37
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	14	1.37
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG21	2	1.37
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG22	2	1.37
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG23	2	1.37
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG21	2	1.37
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG22	2	1.37
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG23	2	1.37
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG21	2	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG22	2	1.37
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG23	2	1.37
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	6	1.37
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	6	1.37
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	6	1.37
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	6	1.37
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	6	1.37
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	6	1.37
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	6	1.37
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	6	1.37
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	6	1.37
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	15	1.36
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	15	1.36
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	15	1.36
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	1	1.36
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	1	1.36
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	1	1.36
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	9	1.35
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	9	1.35
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	9	1.35
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	9	1.35
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	9	1.35
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	9	1.35
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	9	1.35
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	9	1.35
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	9	1.35
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD21	6	1.35
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD22	6	1.35
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD23	6	1.35
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD21	6	1.35
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD22	6	1.35
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD23	6	1.35
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD21	6	1.35
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD22	6	1.35
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD23	6	1.35
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG11	8	1.35
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG12	8	1.35
(1,322)	1:97:A:VAL:HG21	1:179:A:VAL:HG13	8	1.35
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG11	8	1.35
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG12	8	1.35
(1,322)	1:97:A:VAL:HG22	1:179:A:VAL:HG13	8	1.35
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG11	8	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG12	8	1.35
(1,322)	1:97:A:VAL:HG23	1:179:A:VAL:HG13	8	1.35
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	8	1.33
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	8	1.33
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	8	1.33
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	8	1.33
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	8	1.33
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	8	1.33
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	8	1.33
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	8	1.33
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	8	1.33
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD11	13	1.33
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD12	13	1.33
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD13	13	1.33
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD11	13	1.33
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD12	13	1.33
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD13	13	1.33
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD11	13	1.33
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD12	13	1.33
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD13	13	1.33
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD11	14	1.31
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD12	14	1.31
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD13	14	1.31
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD11	14	1.31
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD12	14	1.31
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD13	14	1.31
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD11	14	1.31
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD12	14	1.31
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD13	14	1.31
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD21	14	1.31
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD22	14	1.31
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD23	14	1.31
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD21	14	1.31
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD22	14	1.31
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD23	14	1.31
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD21	14	1.31
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD22	14	1.31
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD23	14	1.31
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG21	5	1.31
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG22	5	1.31
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG23	5	1.31
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG21	5	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG22	5	1.31
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG23	5	1.31
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG21	5	1.31
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG22	5	1.31
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG23	5	1.31
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD11	14	1.31
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD12	14	1.31
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD13	14	1.31
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD11	14	1.31
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD12	14	1.31
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD13	14	1.31
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD11	14	1.31
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD12	14	1.31
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD13	14	1.31
(1,385)	1:207:A:VAL:HG21	1:162:A:THR:H	4	1.3
(1,385)	1:207:A:VAL:HG22	1:162:A:THR:H	4	1.3
(1,385)	1:207:A:VAL:HG23	1:162:A:THR:H	4	1.3
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	9	1.3
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	9	1.3
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	9	1.3
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD11	8	1.3
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD12	8	1.3
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD13	8	1.3
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD11	8	1.3
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD12	8	1.3
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD13	8	1.3
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD11	8	1.3
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD12	8	1.3
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD13	8	1.3
(1,391)	1:217:A:LEU:HD11	1:204:A:LEU:H	15	1.29
(1,391)	1:217:A:LEU:HD12	1:204:A:LEU:H	15	1.29
(1,391)	1:217:A:LEU:HD13	1:204:A:LEU:H	15	1.29
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	2	1.29
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	2	1.29
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	2	1.29
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	9	1.29
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	9	1.29
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	9	1.29
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	9	1.29
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	9	1.29
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	9	1.29
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	9	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	9	1.29
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	9	1.29
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD11	7	1.28
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD12	7	1.28
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD13	7	1.28
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD11	7	1.28
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD12	7	1.28
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD13	7	1.28
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD11	7	1.28
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD12	7	1.28
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD13	7	1.28
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD21	7	1.28
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD22	7	1.28
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD23	7	1.28
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD21	7	1.28
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD22	7	1.28
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD23	7	1.28
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD21	7	1.28
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD22	7	1.28
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD23	7	1.28
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD11	3	1.27
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD12	3	1.27
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD13	3	1.27
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD11	3	1.27
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD12	3	1.27
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD13	3	1.27
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD11	3	1.27
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD12	3	1.27
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD13	3	1.27
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD11	14	1.27
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD12	14	1.27
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD13	14	1.27
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD11	14	1.27
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD12	14	1.27
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD13	14	1.27
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD11	14	1.27
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD12	14	1.27
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD13	14	1.27
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	5	1.27
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	5	1.27
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	5	1.27
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	12	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	8	1.26
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	8	1.26
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	8	1.26
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	8	1.26
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	8	1.26
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	8	1.26
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	8	1.26
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	8	1.26
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	8	1.26
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG21	15	1.25
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG22	15	1.25
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG23	15	1.25
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG21	15	1.25
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG22	15	1.25
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG23	15	1.25
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG21	15	1.25
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG22	15	1.25
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG23	15	1.25
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	11	1.25
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	11	1.25
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	11	1.25
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	13	1.25
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	13	1.25
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	13	1.25
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD11	2	1.25
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD12	2	1.25
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD13	2	1.25
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD11	2	1.25
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD12	2	1.25
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD13	2	1.25
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD11	2	1.25
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD12	2	1.25
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD13	2	1.25
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD21	2	1.25
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD22	2	1.25
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD23	2	1.25
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD21	2	1.25
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD22	2	1.25
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD23	2	1.25
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD21	2	1.25
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD22	2	1.25
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD23	2	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	7	1.25
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	7	1.25
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	7	1.25
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	7	1.25
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	7	1.25
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	7	1.25
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	7	1.25
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	7	1.25
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	7	1.25
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG21	13	1.24
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG22	13	1.24
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG23	13	1.24
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG21	13	1.24
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG22	13	1.24
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG23	13	1.24
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG21	13	1.24
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG22	13	1.24
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG23	13	1.24
(1,351)	1:167:A:LEU:HD11	1:124:A:ILE:H	9	1.24
(1,351)	1:167:A:LEU:HD12	1:124:A:ILE:H	9	1.24
(1,351)	1:167:A:LEU:HD13	1:124:A:ILE:H	9	1.24
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	12	1.24
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	12	1.24
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	12	1.24
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	12	1.24
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	12	1.24
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	12	1.24
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	12	1.24
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	12	1.24
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	12	1.24
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	2	1.24
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	6	1.23
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	6	1.23
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	6	1.23
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	6	1.23
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	6	1.23
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	6	1.23
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	6	1.23
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	6	1.23
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	6	1.23
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD11	15	1.21
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD12	15	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD13	15	1.21
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD11	15	1.21
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD12	15	1.21
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD13	15	1.21
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD11	15	1.21
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD12	15	1.21
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD13	15	1.21
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD21	15	1.21
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD22	15	1.21
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD23	15	1.21
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD21	15	1.21
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD22	15	1.21
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD23	15	1.21
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD21	15	1.21
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD22	15	1.21
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD23	15	1.21
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD11	13	1.21
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD12	13	1.21
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD13	13	1.21
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD11	13	1.21
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD12	13	1.21
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD13	13	1.21
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD11	13	1.21
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD12	13	1.21
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD13	13	1.21
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	7	1.21
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	15	1.2
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	5	1.19
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	5	1.19
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	5	1.19
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD21	8	1.19
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD22	8	1.19
(1,359)	1:177:A:VAL:HG11	1:194:A:LEU:HD23	8	1.19
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD21	8	1.19
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD22	8	1.19
(1,359)	1:177:A:VAL:HG12	1:194:A:LEU:HD23	8	1.19
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD21	8	1.19
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD22	8	1.19
(1,359)	1:177:A:VAL:HG13	1:194:A:LEU:HD23	8	1.19
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	9	1.19
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	11	1.18
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	11	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	11	1.18
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	11	1.18
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	11	1.18
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	11	1.18
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	11	1.18
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	11	1.18
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	11	1.18
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	6	1.18
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	6	1.18
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	6	1.18
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	6	1.18
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	6	1.18
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	6	1.18
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	6	1.18
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	6	1.18
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	6	1.18
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	4	1.18
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	11	1.17
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD11	11	1.16
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD12	11	1.16
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD13	11	1.16
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD11	11	1.16
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD12	11	1.16
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD13	11	1.16
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD11	11	1.16
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD12	11	1.16
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD13	11	1.16
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD21	11	1.16
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD22	11	1.16
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD23	11	1.16
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD21	11	1.16
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD22	11	1.16
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD23	11	1.16
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD21	11	1.16
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD22	11	1.16
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD23	11	1.16
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	4	1.15
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	4	1.15
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	4	1.15
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD11	14	1.14
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD12	14	1.14
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD13	14	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD11	14	1.14
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD12	14	1.14
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD13	14	1.14
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD11	14	1.14
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD12	14	1.14
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD13	14	1.14
(1,319)	1:89:A:LEU:HD11	1:95:A:ASN:H	12	1.14
(1,319)	1:89:A:LEU:HD12	1:95:A:ASN:H	12	1.14
(1,319)	1:89:A:LEU:HD13	1:95:A:ASN:H	12	1.14
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG21	7	1.13
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG22	7	1.13
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG23	7	1.13
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG21	7	1.13
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG22	7	1.13
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG23	7	1.13
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG21	7	1.13
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG22	7	1.13
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG23	7	1.13
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD11	7	1.13
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD12	7	1.13
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD13	7	1.13
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD11	7	1.13
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD12	7	1.13
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD13	7	1.13
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD11	7	1.13
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD12	7	1.13
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD13	7	1.13
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD11	11	1.13
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD12	11	1.13
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD13	11	1.13
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD11	11	1.13
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD12	11	1.13
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD13	11	1.13
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD11	11	1.13
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD12	11	1.13
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD13	11	1.13
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD21	11	1.13
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD22	11	1.13
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD23	11	1.13
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD21	11	1.13
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD22	11	1.13
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD23	11	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD21	11	1.13
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD22	11	1.13
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD23	11	1.13
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	6	1.13
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	6	1.13
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	6	1.13
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	6	1.13
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	6	1.13
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	6	1.13
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	6	1.13
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	6	1.13
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	6	1.13
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD21	8	1.13
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD22	8	1.13
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD23	8	1.13
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD21	8	1.13
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD22	8	1.13
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD23	8	1.13
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD21	8	1.13
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD22	8	1.13
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD23	8	1.13
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	8	1.13
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG21	9	1.12
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG22	9	1.12
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG23	9	1.12
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG21	9	1.12
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG22	9	1.12
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG23	9	1.12
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG21	9	1.12
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG22	9	1.12
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG23	9	1.12
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD11	2	1.12
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD12	2	1.12
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD13	2	1.12
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD11	2	1.12
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD12	2	1.12
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD13	2	1.12
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD11	2	1.12
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD12	2	1.12
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD13	2	1.12
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	6	1.12
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	6	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	6	1.12
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG21	3	1.11
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG22	3	1.11
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG23	3	1.11
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG21	3	1.11
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG22	3	1.11
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG23	3	1.11
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG21	3	1.11
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG22	3	1.11
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG23	3	1.11
(1,324)	1:101:A:LEU:HD11	1:192:A:LEU:HD11	9	1.11
(1,324)	1:101:A:LEU:HD11	1:192:A:LEU:HD12	9	1.11
(1,324)	1:101:A:LEU:HD11	1:192:A:LEU:HD13	9	1.11
(1,324)	1:101:A:LEU:HD12	1:192:A:LEU:HD11	9	1.11
(1,324)	1:101:A:LEU:HD12	1:192:A:LEU:HD12	9	1.11
(1,324)	1:101:A:LEU:HD12	1:192:A:LEU:HD13	9	1.11
(1,324)	1:101:A:LEU:HD13	1:192:A:LEU:HD11	9	1.11
(1,324)	1:101:A:LEU:HD13	1:192:A:LEU:HD12	9	1.11
(1,324)	1:101:A:LEU:HD13	1:192:A:LEU:HD13	9	1.11
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	3	1.1
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	3	1.1
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	3	1.1
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	4	1.1
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	4	1.1
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	4	1.1
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	4	1.1
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	4	1.1
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	4	1.1
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	4	1.1
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	4	1.1
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	4	1.1
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	1	1.1
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	1	1.1
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	1	1.1
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	14	1.09
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	14	1.09
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	14	1.09
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD21	14	1.09
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD22	14	1.09
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD23	14	1.09
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD21	14	1.09
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD22	14	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD23	14	1.09
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD21	14	1.09
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD22	14	1.09
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD23	14	1.09
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	14	1.09
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD21	10	1.08
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD22	10	1.08
(1,394)	1:233:A:THR:HG21	1:194:A:LEU:HD23	10	1.08
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD21	10	1.08
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD22	10	1.08
(1,394)	1:233:A:THR:HG22	1:194:A:LEU:HD23	10	1.08
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD21	10	1.08
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD22	10	1.08
(1,394)	1:233:A:THR:HG23	1:194:A:LEU:HD23	10	1.08
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG21	15	1.08
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG22	15	1.08
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG23	15	1.08
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG21	15	1.08
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG22	15	1.08
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG23	15	1.08
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG21	15	1.08
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG22	15	1.08
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG23	15	1.08
(1,325)	1:101:A:LEU:HD21	1:194:A:LEU:HD21	4	1.08
(1,325)	1:101:A:LEU:HD21	1:194:A:LEU:HD22	4	1.08
(1,325)	1:101:A:LEU:HD21	1:194:A:LEU:HD23	4	1.08
(1,325)	1:101:A:LEU:HD22	1:194:A:LEU:HD21	4	1.08
(1,325)	1:101:A:LEU:HD22	1:194:A:LEU:HD22	4	1.08
(1,325)	1:101:A:LEU:HD22	1:194:A:LEU:HD23	4	1.08
(1,325)	1:101:A:LEU:HD23	1:194:A:LEU:HD21	4	1.08
(1,325)	1:101:A:LEU:HD23	1:194:A:LEU:HD22	4	1.08
(1,325)	1:101:A:LEU:HD23	1:194:A:LEU:HD23	4	1.08
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	1	1.08
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	13	1.07
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	13	1.07
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	13	1.07
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	13	1.06
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	13	1.06
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	13	1.06
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	13	1.06
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	13	1.06
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	13	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	13	1.06
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	13	1.06
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	13	1.06
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	10	1.06
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	10	1.06
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	10	1.06
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	10	1.06
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	10	1.06
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	10	1.06
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	10	1.06
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	10	1.06
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	10	1.06
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	10	1.06
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	10	1.06
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	10	1.06
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	10	1.06
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	10	1.06
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	10	1.06
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	10	1.06
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	10	1.06
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	10	1.06
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	3	1.06
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	3	1.06
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	3	1.06
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	3	1.06
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	3	1.06
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	3	1.06
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	3	1.06
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	3	1.06
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	3	1.06
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD11	10	1.06
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD12	10	1.06
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD13	10	1.06
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD11	10	1.06
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD12	10	1.06
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD13	10	1.06
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD11	10	1.06
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD12	10	1.06
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD13	10	1.06
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	12	1.05
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	12	1.05
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	12	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	12	1.05
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	12	1.05
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	12	1.05
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	12	1.05
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	12	1.05
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	12	1.05
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG21	4	1.05
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG22	4	1.05
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG23	4	1.05
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG21	4	1.05
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG22	4	1.05
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG23	4	1.05
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG21	4	1.05
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG22	4	1.05
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG23	4	1.05
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	14	1.05
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	14	1.05
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	14	1.05
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	14	1.05
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	14	1.05
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	14	1.05
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	14	1.05
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	14	1.05
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	14	1.05
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	2	1.04
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	2	1.04
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	2	1.04
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	4	1.03
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	4	1.03
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	4	1.03
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	6	1.02
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	6	1.02
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	6	1.02
(1,385)	1:207:A:VAL:HG21	1:162:A:THR:H	8	1.02
(1,385)	1:207:A:VAL:HG22	1:162:A:THR:H	8	1.02
(1,385)	1:207:A:VAL:HG23	1:162:A:THR:H	8	1.02
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	3	1.02
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	3	1.02
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	3	1.02
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	2	1.02
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	2	1.02
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	2	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	2	1.02
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	2	1.02
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	2	1.02
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	2	1.02
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	2	1.02
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	2	1.02
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	9	1.02
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	9	1.02
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	9	1.02
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	9	1.02
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	9	1.02
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	9	1.02
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	9	1.02
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	9	1.02
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	9	1.02
(1,345)	1:163:A:LEU:HD11	1:157:A:LEU:H	3	1.02
(1,345)	1:163:A:LEU:HD12	1:157:A:LEU:H	3	1.02
(1,345)	1:163:A:LEU:HD13	1:157:A:LEU:H	3	1.02
(1,345)	1:163:A:LEU:HD11	1:157:A:LEU:H	13	1.02
(1,345)	1:163:A:LEU:HD12	1:157:A:LEU:H	13	1.02
(1,345)	1:163:A:LEU:HD13	1:157:A:LEU:H	13	1.02
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD11	4	1.0
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD12	4	1.0
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD13	4	1.0
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD11	4	1.0
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD12	4	1.0
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD13	4	1.0
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD11	4	1.0
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD12	4	1.0
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD13	4	1.0
(1,385)	1:207:A:VAL:HG21	1:162:A:THR:H	5	1.0
(1,385)	1:207:A:VAL:HG22	1:162:A:THR:H	5	1.0
(1,385)	1:207:A:VAL:HG23	1:162:A:THR:H	5	1.0
(1,351)	1:167:A:LEU:HD11	1:124:A:ILE:H	1	1.0
(1,351)	1:167:A:LEU:HD12	1:124:A:ILE:H	1	1.0
(1,351)	1:167:A:LEU:HD13	1:124:A:ILE:H	1	1.0
(1,344)	1:163:A:LEU:HD21	1:206:A:LYS:H	8	1.0
(1,344)	1:163:A:LEU:HD22	1:206:A:LYS:H	8	1.0
(1,344)	1:163:A:LEU:HD23	1:206:A:LYS:H	8	1.0
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	1	1.0
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	1	1.0
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	1	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	1	1.0
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	1	1.0
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	1	1.0
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	1	1.0
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	1	1.0
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	1	1.0
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	5	1.0
(1,378)	1:195:A:VAL:HG11	1:225:A:ILE:H	15	0.99
(1,378)	1:195:A:VAL:HG12	1:225:A:ILE:H	15	0.99
(1,378)	1:195:A:VAL:HG13	1:225:A:ILE:H	15	0.99
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	13	0.98
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD11	5	0.97
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD12	5	0.97
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD13	5	0.97
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD11	5	0.97
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD12	5	0.97
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD13	5	0.97
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD11	5	0.97
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD12	5	0.97
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD13	5	0.97
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	7	0.95
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	7	0.95
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	7	0.95
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	13	0.95
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	13	0.95
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	13	0.95
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	13	0.95
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	13	0.95
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	13	0.95
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	13	0.95
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	13	0.95
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	13	0.95
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD11	10	0.94
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD12	10	0.94
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD13	10	0.94
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD11	10	0.94
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD12	10	0.94
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD13	10	0.94
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD11	10	0.94
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD12	10	0.94
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD13	10	0.94
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD11	5	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD12	5	0.94
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD13	5	0.94
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD11	5	0.94
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD12	5	0.94
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD13	5	0.94
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD11	5	0.94
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD12	5	0.94
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD13	5	0.94
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD21	5	0.94
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD22	5	0.94
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD23	5	0.94
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD21	5	0.94
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD22	5	0.94
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD23	5	0.94
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD21	5	0.94
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD22	5	0.94
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD23	5	0.94
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	10	0.94
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	3	0.94
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	10	0.94
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	5	0.93
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	5	0.93
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	5	0.93
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	5	0.93
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	5	0.93
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	5	0.93
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	5	0.93
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	5	0.93
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	5	0.93
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	10	0.93
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	10	0.93
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	10	0.93
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	10	0.93
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	10	0.93
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	10	0.93
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	10	0.93
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	10	0.93
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	10	0.93
(1,382)	1:205:A:ILE:HG21	1:216:A:THR:H	12	0.92
(1,382)	1:205:A:ILE:HG22	1:216:A:THR:H	12	0.92
(1,382)	1:205:A:ILE:HG23	1:216:A:THR:H	12	0.92
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG11	14	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG12	14	0.92
(1,355)	1:173:A:VAL:HG11	1:222:A:VAL:HG13	14	0.92
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG11	14	0.92
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG12	14	0.92
(1,355)	1:173:A:VAL:HG12	1:222:A:VAL:HG13	14	0.92
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG11	14	0.92
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG12	14	0.92
(1,355)	1:173:A:VAL:HG13	1:222:A:VAL:HG13	14	0.92
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG11	2	0.92
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG12	2	0.92
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG13	2	0.92
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG11	2	0.92
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG12	2	0.92
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG13	2	0.92
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG11	2	0.92
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG12	2	0.92
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG13	2	0.92
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	6	0.92
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	1	0.92
(1,378)	1:195:A:VAL:HG11	1:225:A:ILE:H	6	0.91
(1,378)	1:195:A:VAL:HG12	1:225:A:ILE:H	6	0.91
(1,378)	1:195:A:VAL:HG13	1:225:A:ILE:H	6	0.91
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	10	0.91
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	10	0.91
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	10	0.91
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	10	0.91
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	10	0.91
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	10	0.91
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	10	0.91
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	10	0.91
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	10	0.91
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG21	2	0.9
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG22	2	0.9
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG23	2	0.9
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG21	2	0.9
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG22	2	0.9
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG23	2	0.9
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG21	2	0.9
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG22	2	0.9
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG23	2	0.9
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD11	7	0.9
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD12	7	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD13	7	0.9
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD11	7	0.9
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD12	7	0.9
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD13	7	0.9
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD11	7	0.9
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD12	7	0.9
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD13	7	0.9
(1,386)	1:207:A:VAL:HG21	1:163:A:LEU:HD21	9	0.9
(1,386)	1:207:A:VAL:HG21	1:163:A:LEU:HD22	9	0.9
(1,386)	1:207:A:VAL:HG21	1:163:A:LEU:HD23	9	0.9
(1,386)	1:207:A:VAL:HG22	1:163:A:LEU:HD21	9	0.9
(1,386)	1:207:A:VAL:HG22	1:163:A:LEU:HD22	9	0.9
(1,386)	1:207:A:VAL:HG22	1:163:A:LEU:HD23	9	0.9
(1,386)	1:207:A:VAL:HG23	1:163:A:LEU:HD21	9	0.9
(1,386)	1:207:A:VAL:HG23	1:163:A:LEU:HD22	9	0.9
(1,386)	1:207:A:VAL:HG23	1:163:A:LEU:HD23	9	0.9
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD21	9	0.9
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD22	9	0.9
(1,364)	1:182:A:ILE:HD11	1:228:A:LEU:HD23	9	0.9
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD21	9	0.9
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD22	9	0.9
(1,364)	1:182:A:ILE:HD12	1:228:A:LEU:HD23	9	0.9
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD21	9	0.9
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD22	9	0.9
(1,364)	1:182:A:ILE:HD13	1:228:A:LEU:HD23	9	0.9
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG11	15	0.9
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG12	15	0.9
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG13	15	0.9
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG11	15	0.9
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG12	15	0.9
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG13	15	0.9
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG11	15	0.9
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG12	15	0.9
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG13	15	0.9
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	5	0.89
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	1	0.88
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	1	0.88
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	1	0.88
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	1	0.88
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	1	0.88
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	1	0.88
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	1	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	1	0.88
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	1	0.88
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	13	0.88
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	13	0.88
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	13	0.88
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	13	0.88
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	13	0.88
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	13	0.88
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	13	0.88
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	13	0.88
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	13	0.88
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	3	0.87
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	3	0.87
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	3	0.87
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	15	0.87
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	15	0.87
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	15	0.87
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	15	0.87
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	15	0.87
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	15	0.87
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	15	0.87
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	15	0.87
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	15	0.87
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD11	15	0.87
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD12	15	0.87
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD13	15	0.87
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD11	15	0.87
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD12	15	0.87
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD13	15	0.87
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD11	15	0.87
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD12	15	0.87
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD13	15	0.87
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD11	6	0.86
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD12	6	0.86
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD13	6	0.86
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD11	6	0.86
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD12	6	0.86
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD13	6	0.86
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD11	6	0.86
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD12	6	0.86
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD13	6	0.86
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG21	6	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG22	6	0.86
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG23	6	0.86
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG21	6	0.86
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG22	6	0.86
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG23	6	0.86
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG21	6	0.86
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG22	6	0.86
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG23	6	0.86
(1,382)	1:205:A:ILE:HG21	1:216:A:THR:H	3	0.86
(1,382)	1:205:A:ILE:HG22	1:216:A:THR:H	3	0.86
(1,382)	1:205:A:ILE:HG23	1:216:A:THR:H	3	0.86
(1,358)	1:176:A:LEU:HD11	1:196:A:TYR:H	2	0.86
(1,358)	1:176:A:LEU:HD12	1:196:A:TYR:H	2	0.86
(1,358)	1:176:A:LEU:HD13	1:196:A:TYR:H	2	0.86
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	10	0.86
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	10	0.86
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	10	0.86
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	10	0.86
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	10	0.86
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	10	0.86
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	10	0.86
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	10	0.86
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	10	0.86
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG21	8	0.86
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG22	8	0.86
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG23	8	0.86
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG21	8	0.86
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG22	8	0.86
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG23	8	0.86
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG21	8	0.86
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG22	8	0.86
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG23	8	0.86
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	5	0.85
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	5	0.85
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	5	0.85
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	5	0.85
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	5	0.85
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	5	0.85
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	5	0.85
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	5	0.85
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	5	0.85
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	8	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	8	0.85
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	8	0.85
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	8	0.84
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	14	0.84
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD11	13	0.83
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD12	13	0.83
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD13	13	0.83
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD11	13	0.83
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD12	13	0.83
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD13	13	0.83
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD11	13	0.83
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD12	13	0.83
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD13	13	0.83
(1,358)	1:176:A:LEU:HD11	1:196:A:TYR:H	6	0.83
(1,358)	1:176:A:LEU:HD12	1:196:A:TYR:H	6	0.83
(1,358)	1:176:A:LEU:HD13	1:196:A:TYR:H	6	0.83
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	9	0.83
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD11	12	0.82
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD12	12	0.82
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD13	12	0.82
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD11	12	0.82
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD12	12	0.82
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD13	12	0.82
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD11	12	0.82
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD12	12	0.82
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD13	12	0.82
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD11	8	0.82
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD12	8	0.82
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD13	8	0.82
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD11	8	0.82
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD12	8	0.82
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD13	8	0.82
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD11	8	0.82
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD12	8	0.82
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD13	8	0.82
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	3	0.82
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD11	9	0.81
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD12	9	0.81
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD13	9	0.81
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD11	9	0.81
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD12	9	0.81
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD13	9	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD11	9	0.81
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD12	9	0.81
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD13	9	0.81
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	7	0.81
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	7	0.81
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	7	0.81
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	7	0.81
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	7	0.81
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	7	0.81
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	7	0.81
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	7	0.81
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	7	0.81
(1,395)	1:237:A:ILE:HD11	1:228:A:LEU:H	10	0.8
(1,395)	1:237:A:ILE:HD12	1:228:A:LEU:H	10	0.8
(1,395)	1:237:A:ILE:HD13	1:228:A:LEU:H	10	0.8
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	15	0.8
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG21	11	0.79
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG22	11	0.79
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG23	11	0.79
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG21	11	0.79
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG22	11	0.79
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG23	11	0.79
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG21	11	0.79
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG22	11	0.79
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG23	11	0.79
(1,352)	1:167:A:LEU:HD21	1:202:A:GLN:H	15	0.79
(1,352)	1:167:A:LEU:HD22	1:202:A:GLN:H	15	0.79
(1,352)	1:167:A:LEU:HD23	1:202:A:GLN:H	15	0.79
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD11	9	0.79
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD12	9	0.79
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD13	9	0.79
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD11	9	0.79
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD12	9	0.79
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD13	9	0.79
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD11	9	0.79
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD12	9	0.79
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD13	9	0.79
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	6	0.79
(1,155)	1:179:A:VAL:H	1:180:A:GLN:H	13	0.79
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG21	11	0.78
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG22	11	0.78
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG23	11	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG21	11	0.78
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG22	11	0.78
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG23	11	0.78
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG21	11	0.78
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG22	11	0.78
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG23	11	0.78
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	11	0.78
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG11	1	0.77
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG12	1	0.77
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG13	1	0.77
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG11	1	0.77
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG12	1	0.77
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG13	1	0.77
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG11	1	0.77
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG12	1	0.77
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG13	1	0.77
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	2	0.77
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD21	13	0.76
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD22	13	0.76
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD23	13	0.76
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD21	13	0.76
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD22	13	0.76
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD23	13	0.76
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD21	13	0.76
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD22	13	0.76
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD23	13	0.76
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	4	0.76
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	7	0.76
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG21	10	0.75
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG22	10	0.75
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG23	10	0.75
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG21	10	0.75
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG22	10	0.75
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG23	10	0.75
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG21	10	0.75
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG22	10	0.75
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG23	10	0.75
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD11	8	0.74
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD12	8	0.74
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD13	8	0.74
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD11	8	0.74
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD12	8	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD13	8	0.74
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD11	8	0.74
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD12	8	0.74
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD13	8	0.74
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD11	9	0.74
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD12	9	0.74
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD13	9	0.74
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD11	9	0.74
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD12	9	0.74
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD13	9	0.74
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD11	9	0.74
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD12	9	0.74
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD13	9	0.74
(1,396)	1:237:A:ILE:HD11	1:229:A:CYS:H	14	0.73
(1,396)	1:237:A:ILE:HD12	1:229:A:CYS:H	14	0.73
(1,396)	1:237:A:ILE:HD13	1:229:A:CYS:H	14	0.73
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	10	0.73
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	10	0.73
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	10	0.73
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	2	0.73
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	2	0.73
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	2	0.73
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	2	0.73
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	2	0.73
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	2	0.73
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	2	0.73
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	2	0.73
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	2	0.73
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD11	3	0.73
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD12	3	0.73
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD13	3	0.73
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD11	3	0.73
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD12	3	0.73
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD13	3	0.73
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD11	3	0.73
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD12	3	0.73
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD13	3	0.73
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	7	0.72
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	7	0.72
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	7	0.72
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	11	0.72
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	11	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	11	0.72
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	11	0.72
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	11	0.72
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	11	0.72
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	11	0.72
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	11	0.72
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	11	0.72
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB1	5	0.71
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB2	5	0.71
(1,369)	1:189:A:LEU:HD21	1:231:A:ALA:HB3	5	0.71
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB1	5	0.71
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB2	5	0.71
(1,369)	1:189:A:LEU:HD22	1:231:A:ALA:HB3	5	0.71
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB1	5	0.71
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB2	5	0.71
(1,369)	1:189:A:LEU:HD23	1:231:A:ALA:HB3	5	0.71
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	14	0.71
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	14	0.71
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	14	0.71
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	14	0.71
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	14	0.71
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	14	0.71
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	14	0.71
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	14	0.71
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	14	0.71
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	4	0.7
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	4	0.7
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	4	0.7
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD11	15	0.7
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD12	15	0.7
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD13	15	0.7
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD11	15	0.7
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD12	15	0.7
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD13	15	0.7
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD11	15	0.7
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD12	15	0.7
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD13	15	0.7
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD11	2	0.69
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD12	2	0.69
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD13	2	0.69
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD11	2	0.69
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD12	2	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD13	2	0.69
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD11	2	0.69
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD12	2	0.69
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD13	2	0.69
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	7	0.69
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	7	0.69
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	7	0.69
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	7	0.69
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	7	0.69
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	7	0.69
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	7	0.69
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	7	0.69
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	7	0.69
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	5	0.68
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	5	0.68
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	5	0.68
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	5	0.68
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	5	0.68
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	5	0.68
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	5	0.68
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	5	0.68
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	5	0.68
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD11	13	0.68
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD12	13	0.68
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD13	13	0.68
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD11	13	0.68
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD12	13	0.68
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD13	13	0.68
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD11	13	0.68
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD12	13	0.68
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD13	13	0.68
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD11	7	0.67
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD12	7	0.67
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD13	7	0.67
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD11	7	0.67
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD12	7	0.67
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD13	7	0.67
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD11	7	0.67
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD12	7	0.67
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD13	7	0.67
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD21	7	0.67
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD22	7	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD23	7	0.67
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD21	7	0.67
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD22	7	0.67
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD23	7	0.67
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD21	7	0.67
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD22	7	0.67
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD23	7	0.67
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	4	0.67
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	4	0.67
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	4	0.67
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	4	0.67
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	4	0.67
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	4	0.67
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	4	0.67
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	4	0.67
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	4	0.67
(1,157)	1:179:A:VAL:HA	1:180:A:GLN:H	12	0.67
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	4	0.65
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	4	0.65
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	4	0.65
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG21	6	0.64
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG22	6	0.64
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG23	6	0.64
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG21	6	0.64
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG22	6	0.64
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG23	6	0.64
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG21	6	0.64
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG22	6	0.64
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG23	6	0.64
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	15	0.64
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	15	0.64
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	15	0.64
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	5	0.64
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	5	0.64
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	5	0.64
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	9	0.64
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	9	0.64
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	9	0.64
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD11	5	0.63
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD12	5	0.63
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD13	5	0.63
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD11	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD12	5	0.63
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD13	5	0.63
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD11	5	0.63
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD12	5	0.63
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD13	5	0.63
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD21	5	0.63
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD22	5	0.63
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD23	5	0.63
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD21	5	0.63
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD22	5	0.63
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD23	5	0.63
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD21	5	0.63
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD22	5	0.63
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD23	5	0.63
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD11	10	0.63
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD12	10	0.63
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD13	10	0.63
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD11	10	0.63
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD12	10	0.63
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD13	10	0.63
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD11	10	0.63
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD12	10	0.63
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD13	10	0.63
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD21	10	0.63
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD22	10	0.63
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD23	10	0.63
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD21	10	0.63
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD22	10	0.63
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD23	10	0.63
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD21	10	0.63
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD22	10	0.63
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD23	10	0.63
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD11	8	0.63
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD12	8	0.63
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD13	8	0.63
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD11	8	0.63
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD12	8	0.63
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD13	8	0.63
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD11	8	0.63
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD12	8	0.63
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD13	8	0.63
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG21	7	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG22	7	0.63
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG23	7	0.63
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG21	7	0.63
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG22	7	0.63
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG23	7	0.63
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG21	7	0.63
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG22	7	0.63
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG23	7	0.63
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	11	0.62
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	11	0.62
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	11	0.62
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	11	0.62
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	11	0.62
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	11	0.62
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	11	0.62
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	11	0.62
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	11	0.62
(1,345)	1:163:A:LEU:HD11	1:157:A:LEU:H	12	0.62
(1,345)	1:163:A:LEU:HD12	1:157:A:LEU:H	12	0.62
(1,345)	1:163:A:LEU:HD13	1:157:A:LEU:H	12	0.62
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	3	0.62
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	3	0.62
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	3	0.62
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	3	0.62
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	3	0.62
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	3	0.62
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	3	0.62
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	3	0.62
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	3	0.62
(1,319)	1:89:A:LEU:HD11	1:95:A:ASN:H	6	0.62
(1,319)	1:89:A:LEU:HD12	1:95:A:ASN:H	6	0.62
(1,319)	1:89:A:LEU:HD13	1:95:A:ASN:H	6	0.62
(1,393)	1:228:A:LEU:HD11	1:238:A:LEU:H	14	0.61
(1,393)	1:228:A:LEU:HD12	1:238:A:LEU:H	14	0.61
(1,393)	1:228:A:LEU:HD13	1:238:A:LEU:H	14	0.61
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG21	14	0.61
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG22	14	0.61
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG23	14	0.61
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG21	14	0.61
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG22	14	0.61
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG23	14	0.61
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG21	14	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG22	14	0.61
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG23	14	0.61
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	8	0.61
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	8	0.61
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	8	0.61
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	8	0.61
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	8	0.61
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	8	0.61
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	8	0.61
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	8	0.61
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	8	0.61
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG21	4	0.61
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG22	4	0.61
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG23	4	0.61
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG21	4	0.61
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG22	4	0.61
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG23	4	0.61
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG21	4	0.61
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG22	4	0.61
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG23	4	0.61
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	8	0.6
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	8	0.6
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	8	0.6
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	9	0.6
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	9	0.6
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	9	0.6
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	9	0.6
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	9	0.6
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	9	0.6
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	9	0.6
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	9	0.6
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	9	0.6
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD11	4	0.6
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD12	4	0.6
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD13	4	0.6
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD11	4	0.6
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD12	4	0.6
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD13	4	0.6
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD11	4	0.6
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD12	4	0.6
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD13	4	0.6
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD21	4	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD22	4	0.6
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD23	4	0.6
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD21	4	0.6
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD22	4	0.6
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD23	4	0.6
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD21	4	0.6
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD22	4	0.6
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD23	4	0.6
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	13	0.59
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	13	0.59
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	13	0.59
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	13	0.59
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	13	0.59
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	13	0.59
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	13	0.59
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	13	0.59
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	13	0.59
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	15	0.59
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	15	0.59
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	15	0.59
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	15	0.59
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	15	0.59
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	15	0.59
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	15	0.59
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	15	0.59
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	15	0.59
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD11	1	0.58
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD12	1	0.58
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD13	1	0.58
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD11	1	0.58
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD12	1	0.58
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD13	1	0.58
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD11	1	0.58
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD12	1	0.58
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD13	1	0.58
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	3	0.57
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	3	0.57
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	3	0.57
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	3	0.57
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	3	0.57
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	3	0.57
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	3	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	3	0.57
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	3	0.57
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD11	8	0.57
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD12	8	0.57
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD13	8	0.57
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD11	8	0.57
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD12	8	0.57
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD13	8	0.57
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD11	8	0.57
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD12	8	0.57
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD13	8	0.57
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD21	8	0.57
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD22	8	0.57
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD23	8	0.57
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD21	8	0.57
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD22	8	0.57
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD23	8	0.57
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD21	8	0.57
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD22	8	0.57
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD23	8	0.57
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG21	8	0.56
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG22	8	0.56
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG23	8	0.56
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG21	8	0.56
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG22	8	0.56
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG23	8	0.56
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG21	8	0.56
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG22	8	0.56
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG23	8	0.56
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	5	0.56
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	5	0.56
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	5	0.56
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD11	11	0.56
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD12	11	0.56
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD13	11	0.56
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD11	11	0.56
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD12	11	0.56
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD13	11	0.56
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD11	11	0.56
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD12	11	0.56
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD13	11	0.56
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD21	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD22	8	0.55
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD23	8	0.55
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD21	8	0.55
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD22	8	0.55
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD23	8	0.55
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD21	8	0.55
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD22	8	0.55
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD23	8	0.55
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	14	0.54
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	14	0.54
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	14	0.54
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD11	1	0.54
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD12	1	0.54
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD13	1	0.54
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD11	1	0.54
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD12	1	0.54
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD13	1	0.54
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD11	1	0.54
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD12	1	0.54
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD13	1	0.54
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD21	1	0.54
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD22	1	0.54
(1,346)	1:163:A:LEU:HD21	1:204:A:LEU:HD23	1	0.54
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD21	1	0.54
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD22	1	0.54
(1,346)	1:163:A:LEU:HD22	1:204:A:LEU:HD23	1	0.54
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD21	1	0.54
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD22	1	0.54
(1,346)	1:163:A:LEU:HD23	1:204:A:LEU:HD23	1	0.54
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG21	13	0.54
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG22	13	0.54
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG23	13	0.54
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG21	13	0.54
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG22	13	0.54
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG23	13	0.54
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG21	13	0.54
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG22	13	0.54
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG23	13	0.54
(1,378)	1:195:A:VAL:HG11	1:225:A:ILE:H	9	0.53
(1,378)	1:195:A:VAL:HG12	1:225:A:ILE:H	9	0.53
(1,378)	1:195:A:VAL:HG13	1:225:A:ILE:H	9	0.53
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD11	9	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD12	9	0.52
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD13	9	0.52
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD11	9	0.52
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD12	9	0.52
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD13	9	0.52
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD11	9	0.52
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD12	9	0.52
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD13	9	0.52
(1,393)	1:228:A:LEU:HD11	1:238:A:LEU:H	1	0.52
(1,393)	1:228:A:LEU:HD12	1:238:A:LEU:H	1	0.52
(1,393)	1:228:A:LEU:HD13	1:238:A:LEU:H	1	0.52
(1,388)	1:207:A:VAL:HG21	1:161:A:ALA:H	10	0.51
(1,388)	1:207:A:VAL:HG22	1:161:A:ALA:H	10	0.51
(1,388)	1:207:A:VAL:HG23	1:161:A:ALA:H	10	0.51
(1,372)	1:194:A:LEU:HD11	1:228:A:LEU:H	12	0.51
(1,372)	1:194:A:LEU:HD12	1:228:A:LEU:H	12	0.51
(1,372)	1:194:A:LEU:HD13	1:228:A:LEU:H	12	0.51
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	1	0.5
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	1	0.5
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	1	0.5
(1,362)	1:179:A:VAL:HG11	1:97:A:VAL:H	1	0.5
(1,362)	1:179:A:VAL:HG12	1:97:A:VAL:H	1	0.5
(1,362)	1:179:A:VAL:HG13	1:97:A:VAL:H	1	0.5
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	9	0.5
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	9	0.5
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	9	0.5
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	9	0.5
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	9	0.5
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	9	0.5
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	9	0.5
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	9	0.5
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	9	0.5
(1,378)	1:195:A:VAL:HG11	1:225:A:ILE:H	4	0.49
(1,378)	1:195:A:VAL:HG12	1:225:A:ILE:H	4	0.49
(1,378)	1:195:A:VAL:HG13	1:225:A:ILE:H	4	0.49
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	14	0.49
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	14	0.49
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	14	0.49
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	14	0.49
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	14	0.49
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	14	0.49
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	14	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	14	0.49
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	14	0.49
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	13	0.49
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	13	0.49
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	13	0.49
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	13	0.49
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	13	0.49
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	13	0.49
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	13	0.49
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	13	0.49
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	13	0.49
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD11	15	0.48
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD12	15	0.48
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD13	15	0.48
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD11	15	0.48
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD12	15	0.48
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD13	15	0.48
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD11	15	0.48
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD12	15	0.48
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD13	15	0.48
(1,378)	1:195:A:VAL:HG11	1:225:A:ILE:H	11	0.48
(1,378)	1:195:A:VAL:HG12	1:225:A:ILE:H	11	0.48
(1,378)	1:195:A:VAL:HG13	1:225:A:ILE:H	11	0.48
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD11	15	0.48
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD12	15	0.48
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD13	15	0.48
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD11	15	0.48
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD12	15	0.48
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD13	15	0.48
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD11	15	0.48
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD12	15	0.48
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD13	15	0.48
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD11	10	0.48
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD12	10	0.48
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD13	10	0.48
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD11	10	0.48
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD12	10	0.48
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD13	10	0.48
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD11	10	0.48
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD12	10	0.48
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD13	10	0.48
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG21	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG22	7	0.47
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG23	7	0.47
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG21	7	0.47
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG22	7	0.47
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG23	7	0.47
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG21	7	0.47
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG22	7	0.47
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG23	7	0.47
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG21	4	0.47
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG22	4	0.47
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG23	4	0.47
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG21	4	0.47
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG22	4	0.47
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG23	4	0.47
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG21	4	0.47
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG22	4	0.47
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG23	4	0.47
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD11	3	0.47
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD12	3	0.47
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD13	3	0.47
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD11	3	0.47
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD12	3	0.47
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD13	3	0.47
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD11	3	0.47
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD12	3	0.47
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD13	3	0.47
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG21	6	0.47
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG22	6	0.47
(1,332)	1:126:A:VAL:HG11	1:122:A:THR:HG23	6	0.47
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG21	6	0.47
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG22	6	0.47
(1,332)	1:126:A:VAL:HG12	1:122:A:THR:HG23	6	0.47
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG21	6	0.47
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG22	6	0.47
(1,332)	1:126:A:VAL:HG13	1:122:A:THR:HG23	6	0.47
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG21	7	0.46
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG22	7	0.46
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG23	7	0.46
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG21	7	0.46
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG22	7	0.46
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG23	7	0.46
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG21	7	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG22	7	0.46
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG23	7	0.46
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	15	0.46
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	15	0.46
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	15	0.46
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD11	10	0.44
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD12	10	0.44
(1,398)	1:238:A:LEU:HD21	1:225:A:ILE:HD13	10	0.44
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD11	10	0.44
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD12	10	0.44
(1,398)	1:238:A:LEU:HD22	1:225:A:ILE:HD13	10	0.44
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD11	10	0.44
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD12	10	0.44
(1,398)	1:238:A:LEU:HD23	1:225:A:ILE:HD13	10	0.44
(1,378)	1:195:A:VAL:HG11	1:225:A:ILE:H	2	0.44
(1,378)	1:195:A:VAL:HG12	1:225:A:ILE:H	2	0.44
(1,378)	1:195:A:VAL:HG13	1:225:A:ILE:H	2	0.44
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD21	9	0.44
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD22	9	0.44
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD23	9	0.44
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD21	9	0.44
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD22	9	0.44
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD23	9	0.44
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD21	9	0.44
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD22	9	0.44
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD23	9	0.44
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG21	8	0.44
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG22	8	0.44
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG23	8	0.44
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG21	8	0.44
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG22	8	0.44
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG23	8	0.44
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG21	8	0.44
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG22	8	0.44
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG23	8	0.44
(1,345)	1:163:A:LEU:HD11	1:157:A:LEU:H	5	0.43
(1,345)	1:163:A:LEU:HD12	1:157:A:LEU:H	5	0.43
(1,345)	1:163:A:LEU:HD13	1:157:A:LEU:H	5	0.43
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD21	5	0.43
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD22	5	0.43
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD23	5	0.43
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD21	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD22	5	0.43
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD23	5	0.43
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD21	5	0.43
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD22	5	0.43
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD23	5	0.43
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD11	11	0.42
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD12	11	0.42
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD13	11	0.42
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD11	11	0.42
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD12	11	0.42
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD13	11	0.42
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD11	11	0.42
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD12	11	0.42
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD13	11	0.42
(1,353)	1:168:A:ILE:HD11	1:202:A:GLN:H	12	0.42
(1,353)	1:168:A:ILE:HD12	1:202:A:GLN:H	12	0.42
(1,353)	1:168:A:ILE:HD13	1:202:A:GLN:H	12	0.42
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB1	1	0.42
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB2	1	0.42
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB3	1	0.42
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB1	1	0.42
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB2	1	0.42
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB3	1	0.42
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB1	1	0.42
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB2	1	0.42
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB3	1	0.42
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB1	1	0.42
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB2	1	0.42
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB3	1	0.42
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB1	1	0.42
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB2	1	0.42
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB3	1	0.42
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB1	1	0.42
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB2	1	0.42
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB3	1	0.42
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	9	0.41
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	9	0.41
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	9	0.41
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD11	4	0.41
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD12	4	0.41
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD13	4	0.41
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD11	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD12	4	0.41
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD13	4	0.41
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD11	4	0.41
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD12	4	0.41
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD13	4	0.41
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD21	15	0.41
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD22	15	0.41
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD23	15	0.41
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD21	15	0.41
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD22	15	0.41
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD23	15	0.41
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD21	15	0.41
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD22	15	0.41
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD23	15	0.41
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD21	3	0.41
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD22	3	0.41
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD23	3	0.41
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD21	3	0.41
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD22	3	0.41
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD23	3	0.41
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD21	3	0.41
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD22	3	0.41
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD23	3	0.41
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD11	15	0.41
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD12	15	0.41
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD13	15	0.41
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD11	15	0.41
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD12	15	0.41
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD13	15	0.41
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD11	15	0.41
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD12	15	0.41
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD13	15	0.41
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG21	13	0.4
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG22	13	0.4
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG23	13	0.4
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG21	13	0.4
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG22	13	0.4
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG23	13	0.4
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG21	13	0.4
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG22	13	0.4
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG23	13	0.4
(1,393)	1:228:A:LEU:HD11	1:238:A:LEU:H	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:228:A:LEU:HD12	1:238:A:LEU:H	2	0.4
(1,393)	1:228:A:LEU:HD13	1:238:A:LEU:H	2	0.4
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	11	0.4
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	11	0.4
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	11	0.4
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD11	3	0.4
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD12	3	0.4
(1,381)	1:204:A:LEU:HD21	1:217:A:LEU:HD13	3	0.4
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD11	3	0.4
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD12	3	0.4
(1,381)	1:204:A:LEU:HD22	1:217:A:LEU:HD13	3	0.4
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD11	3	0.4
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD12	3	0.4
(1,381)	1:204:A:LEU:HD23	1:217:A:LEU:HD13	3	0.4
(1,393)	1:228:A:LEU:HD11	1:238:A:LEU:H	13	0.39
(1,393)	1:228:A:LEU:HD12	1:238:A:LEU:H	13	0.39
(1,393)	1:228:A:LEU:HD13	1:238:A:LEU:H	13	0.39
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	6	0.39
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	6	0.39
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	6	0.39
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	6	0.39
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	6	0.39
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	6	0.39
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	6	0.39
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	6	0.39
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	6	0.39
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG21	4	0.39
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG22	4	0.39
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG23	4	0.39
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG21	4	0.39
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG22	4	0.39
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG23	4	0.39
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG21	4	0.39
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG22	4	0.39
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG23	4	0.39
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG21	2	0.38
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG22	2	0.38
(1,383)	1:205:A:ILE:HG21	1:216:A:THR:HG23	2	0.38
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG21	2	0.38
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG22	2	0.38
(1,383)	1:205:A:ILE:HG22	1:216:A:THR:HG23	2	0.38
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG21	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG22	2	0.38
(1,383)	1:205:A:ILE:HG23	1:216:A:THR:HG23	2	0.38
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG21	5	0.38
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG22	5	0.38
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG23	5	0.38
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG21	5	0.38
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG22	5	0.38
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG23	5	0.38
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG21	5	0.38
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG22	5	0.38
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG23	5	0.38
(1,386)	1:207:A:VAL:HG21	1:163:A:LEU:HD21	15	0.37
(1,386)	1:207:A:VAL:HG21	1:163:A:LEU:HD22	15	0.37
(1,386)	1:207:A:VAL:HG21	1:163:A:LEU:HD23	15	0.37
(1,386)	1:207:A:VAL:HG22	1:163:A:LEU:HD21	15	0.37
(1,386)	1:207:A:VAL:HG22	1:163:A:LEU:HD22	15	0.37
(1,386)	1:207:A:VAL:HG22	1:163:A:LEU:HD23	15	0.37
(1,386)	1:207:A:VAL:HG23	1:163:A:LEU:HD21	15	0.37
(1,386)	1:207:A:VAL:HG23	1:163:A:LEU:HD22	15	0.37
(1,386)	1:207:A:VAL:HG23	1:163:A:LEU:HD23	15	0.37
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG21	8	0.37
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG22	8	0.37
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG23	8	0.37
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG21	8	0.37
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG22	8	0.37
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG23	8	0.37
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG21	8	0.37
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG22	8	0.37
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG23	8	0.37
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD11	6	0.37
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD12	6	0.37
(1,365)	1:182:A:ILE:HD11	1:228:A:LEU:HD13	6	0.37
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD11	6	0.37
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD12	6	0.37
(1,365)	1:182:A:ILE:HD12	1:228:A:LEU:HD13	6	0.37
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD11	6	0.37
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD12	6	0.37
(1,365)	1:182:A:ILE:HD13	1:228:A:LEU:HD13	6	0.37
(1,351)	1:167:A:LEU:HD11	1:124:A:ILE:H	3	0.37
(1,351)	1:167:A:LEU:HD12	1:124:A:ILE:H	3	0.37
(1,351)	1:167:A:LEU:HD13	1:124:A:ILE:H	3	0.37
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD11	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD12	8	0.37
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD13	8	0.37
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD11	8	0.37
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD12	8	0.37
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD13	8	0.37
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD11	8	0.37
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD12	8	0.37
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD13	8	0.37
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD21	9	0.35
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD22	9	0.35
(1,360)	1:177:A:VAL:HG11	1:192:A:LEU:HD23	9	0.35
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD21	9	0.35
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD22	9	0.35
(1,360)	1:177:A:VAL:HG12	1:192:A:LEU:HD23	9	0.35
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD21	9	0.35
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD22	9	0.35
(1,360)	1:177:A:VAL:HG13	1:192:A:LEU:HD23	9	0.35
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD11	5	0.35
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD12	5	0.35
(1,329)	1:124:A:ILE:HG21	1:120:A:ILE:HD13	5	0.35
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD11	5	0.35
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD12	5	0.35
(1,329)	1:124:A:ILE:HG22	1:120:A:ILE:HD13	5	0.35
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD11	5	0.35
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD12	5	0.35
(1,329)	1:124:A:ILE:HG23	1:120:A:ILE:HD13	5	0.35
(1,395)	1:237:A:ILE:HD11	1:228:A:LEU:H	8	0.34
(1,395)	1:237:A:ILE:HD12	1:228:A:LEU:H	8	0.34
(1,395)	1:237:A:ILE:HD13	1:228:A:LEU:H	8	0.34
(1,378)	1:195:A:VAL:HG11	1:225:A:ILE:H	7	0.34
(1,378)	1:195:A:VAL:HG12	1:225:A:ILE:H	7	0.34
(1,378)	1:195:A:VAL:HG13	1:225:A:ILE:H	7	0.34
(1,351)	1:167:A:LEU:HD11	1:124:A:ILE:H	2	0.34
(1,351)	1:167:A:LEU:HD12	1:124:A:ILE:H	2	0.34
(1,351)	1:167:A:LEU:HD13	1:124:A:ILE:H	2	0.34
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	6	0.34
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	6	0.34
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	6	0.34
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	6	0.34
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	6	0.34
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	6	0.34
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	6	0.34
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	6	0.34
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB1	14	0.33
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB2	14	0.33
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB3	14	0.33
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB1	14	0.33
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB2	14	0.33
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB3	14	0.33
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB1	14	0.33
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB2	14	0.33
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB3	14	0.33
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB1	14	0.33
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB2	14	0.33
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB3	14	0.33
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB1	14	0.33
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB2	14	0.33
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB3	14	0.33
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB1	14	0.33
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB2	14	0.33
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB3	14	0.33
(1,392)	1:221:A:VAL:HG11	1:201:A:LYS:H	10	0.32
(1,392)	1:221:A:VAL:HG12	1:201:A:LYS:H	10	0.32
(1,392)	1:221:A:VAL:HG13	1:201:A:LYS:H	10	0.32
(1,352)	1:167:A:LEU:HD21	1:202:A:GLN:H	2	0.32
(1,352)	1:167:A:LEU:HD22	1:202:A:GLN:H	2	0.32
(1,352)	1:167:A:LEU:HD23	1:202:A:GLN:H	2	0.32
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG21	15	0.32
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG22	15	0.32
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG23	15	0.32
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG21	15	0.32
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG22	15	0.32
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG23	15	0.32
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG21	15	0.32
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG22	15	0.32
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG23	15	0.32
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	2	0.3
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	2	0.3
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	2	0.3
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	2	0.3
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	2	0.3
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	2	0.3
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	2	0.3
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	2	0.3
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	3	0.3
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	3	0.3
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	3	0.3
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	3	0.3
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	3	0.3
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	3	0.3
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	3	0.3
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	3	0.3
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	3	0.3
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD11	6	0.3
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD12	6	0.3
(1,328)	1:122:A:THR:HG21	1:141:A:LEU:HD13	6	0.3
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD11	6	0.3
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD12	6	0.3
(1,328)	1:122:A:THR:HG22	1:141:A:LEU:HD13	6	0.3
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD11	6	0.3
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD12	6	0.3
(1,328)	1:122:A:THR:HG23	1:141:A:LEU:HD13	6	0.3
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	5	0.29
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	5	0.29
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	5	0.29
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG21	7	0.29
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG22	7	0.29
(1,356)	1:173:A:VAL:HG11	1:222:A:VAL:HG23	7	0.29
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG21	7	0.29
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG22	7	0.29
(1,356)	1:173:A:VAL:HG12	1:222:A:VAL:HG23	7	0.29
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG21	7	0.29
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG22	7	0.29
(1,356)	1:173:A:VAL:HG13	1:222:A:VAL:HG23	7	0.29
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD11	5	0.29
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD12	5	0.29
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD13	5	0.29
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD11	5	0.29
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD12	5	0.29
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD13	5	0.29
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD11	5	0.29
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD12	5	0.29
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD13	5	0.29
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG21	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG22	8	0.29
(1,342)	1:161:A:ALA:HB1	1:207:A:VAL:HG23	8	0.29
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG21	8	0.29
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG22	8	0.29
(1,342)	1:161:A:ALA:HB2	1:207:A:VAL:HG23	8	0.29
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG21	8	0.29
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG22	8	0.29
(1,342)	1:161:A:ALA:HB3	1:207:A:VAL:HG23	8	0.29
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD21	7	0.29
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD22	7	0.29
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD23	7	0.29
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD21	7	0.29
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD22	7	0.29
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD23	7	0.29
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD21	7	0.29
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD22	7	0.29
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD23	7	0.29
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD11	2	0.28
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD12	2	0.28
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD13	2	0.28
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD11	2	0.28
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD12	2	0.28
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD13	2	0.28
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD11	2	0.28
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD12	2	0.28
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD13	2	0.28
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD21	2	0.28
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD22	2	0.28
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD23	2	0.28
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD21	2	0.28
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD22	2	0.28
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD23	2	0.28
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD21	2	0.28
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD22	2	0.28
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD23	2	0.28
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD11	9	0.27
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD12	9	0.27
(1,367)	1:184:A:ILE:HD11	1:182:A:ILE:HD13	9	0.27
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD11	9	0.27
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD12	9	0.27
(1,367)	1:184:A:ILE:HD12	1:182:A:ILE:HD13	9	0.27
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD11	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD12	9	0.27
(1,367)	1:184:A:ILE:HD13	1:182:A:ILE:HD13	9	0.27
(1,351)	1:167:A:LEU:HD11	1:124:A:ILE:H	14	0.27
(1,351)	1:167:A:LEU:HD12	1:124:A:ILE:H	14	0.27
(1,351)	1:167:A:LEU:HD13	1:124:A:ILE:H	14	0.27
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG21	15	0.27
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG22	15	0.27
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG23	15	0.27
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG21	15	0.27
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG22	15	0.27
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG23	15	0.27
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG21	15	0.27
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG22	15	0.27
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG23	15	0.27
(1,319)	1:89:A:LEU:HD11	1:95:A:ASN:H	9	0.27
(1,319)	1:89:A:LEU:HD12	1:95:A:ASN:H	9	0.27
(1,319)	1:89:A:LEU:HD13	1:95:A:ASN:H	9	0.27
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB1	10	0.27
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB2	10	0.27
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB3	10	0.27
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB1	10	0.27
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB2	10	0.27
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB3	10	0.27
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB1	10	0.27
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB2	10	0.27
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB3	10	0.27
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB1	10	0.27
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB2	10	0.27
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB3	10	0.27
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB1	10	0.27
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB2	10	0.27
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB3	10	0.27
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB1	10	0.27
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB2	10	0.27
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB3	10	0.27
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG21	9	0.26
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG22	9	0.26
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG23	9	0.26
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG21	9	0.26
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG22	9	0.26
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG23	9	0.26
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG21	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG22	9	0.26
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG23	9	0.26
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG21	15	0.26
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG22	15	0.26
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG23	15	0.26
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG21	15	0.26
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG22	15	0.26
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG23	15	0.26
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG21	15	0.26
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG22	15	0.26
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG23	15	0.26
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG21	4	0.26
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG22	4	0.26
(1,347)	1:167:A:LEU:HD11	1:124:A:ILE:HG23	4	0.26
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG21	4	0.26
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG22	4	0.26
(1,347)	1:167:A:LEU:HD12	1:124:A:ILE:HG23	4	0.26
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG21	4	0.26
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG22	4	0.26
(1,347)	1:167:A:LEU:HD13	1:124:A:ILE:HG23	4	0.26
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	11	0.26
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	11	0.26
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	11	0.26
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	11	0.26
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	11	0.26
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	11	0.26
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	11	0.26
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	11	0.26
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	11	0.26
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD21	10	0.26
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD22	10	0.26
(1,337)	1:141:A:LEU:HD11	1:238:A:LEU:HD23	10	0.26
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD21	10	0.26
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD22	10	0.26
(1,337)	1:141:A:LEU:HD12	1:238:A:LEU:HD23	10	0.26
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD21	10	0.26
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD22	10	0.26
(1,337)	1:141:A:LEU:HD13	1:238:A:LEU:HD23	10	0.26
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG11	15	0.25
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG12	15	0.25
(1,357)	1:176:A:LEU:HD11	1:195:A:VAL:HG13	15	0.25
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG11	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG12	15	0.25
(1,357)	1:176:A:LEU:HD12	1:195:A:VAL:HG13	15	0.25
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG11	15	0.25
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG12	15	0.25
(1,357)	1:176:A:LEU:HD13	1:195:A:VAL:HG13	15	0.25
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	10	0.25
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	10	0.25
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	10	0.25
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD11	2	0.25
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD12	2	0.25
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD13	2	0.25
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD11	2	0.25
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD12	2	0.25
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD13	2	0.25
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD11	2	0.25
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD12	2	0.25
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD13	2	0.25
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD21	13	0.25
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD22	13	0.25
(1,331)	1:126:A:VAL:HG11	1:141:A:LEU:HD23	13	0.25
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD21	13	0.25
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD22	13	0.25
(1,331)	1:126:A:VAL:HG12	1:141:A:LEU:HD23	13	0.25
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD21	13	0.25
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD22	13	0.25
(1,331)	1:126:A:VAL:HG13	1:141:A:LEU:HD23	13	0.25
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG11	15	0.25
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG12	15	0.25
(1,320)	1:94:A:LEU:HD11	1:179:A:VAL:HG13	15	0.25
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG11	15	0.25
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG12	15	0.25
(1,320)	1:94:A:LEU:HD12	1:179:A:VAL:HG13	15	0.25
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG11	15	0.25
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG12	15	0.25
(1,320)	1:94:A:LEU:HD13	1:179:A:VAL:HG13	15	0.25
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD11	12	0.24
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD12	12	0.24
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD13	12	0.24
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD11	12	0.24
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD12	12	0.24
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD13	12	0.24
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD11	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD12	12	0.24
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD13	12	0.24
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD21	12	0.24
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD22	12	0.24
(1,397)	1:238:A:LEU:HD11	1:141:A:LEU:HD23	12	0.24
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD21	12	0.24
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD22	12	0.24
(1,397)	1:238:A:LEU:HD12	1:141:A:LEU:HD23	12	0.24
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD21	12	0.24
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD22	12	0.24
(1,397)	1:238:A:LEU:HD13	1:141:A:LEU:HD23	12	0.24
(1,378)	1:195:A:VAL:HG11	1:225:A:ILE:H	5	0.24
(1,378)	1:195:A:VAL:HG12	1:225:A:ILE:H	5	0.24
(1,378)	1:195:A:VAL:HG13	1:225:A:ILE:H	5	0.24
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG21	1	0.24
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG22	1	0.24
(1,321)	1:94:A:LEU:HD11	1:179:A:VAL:HG23	1	0.24
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG21	1	0.24
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG22	1	0.24
(1,321)	1:94:A:LEU:HD12	1:179:A:VAL:HG23	1	0.24
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG21	1	0.24
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG22	1	0.24
(1,321)	1:94:A:LEU:HD13	1:179:A:VAL:HG23	1	0.24
(1,387)	1:207:A:VAL:HG11	1:214:A:THR:H	8	0.23
(1,387)	1:207:A:VAL:HG12	1:214:A:THR:H	8	0.23
(1,387)	1:207:A:VAL:HG13	1:214:A:THR:H	8	0.23
(1,358)	1:176:A:LEU:HD11	1:196:A:TYR:H	5	0.23
(1,358)	1:176:A:LEU:HD12	1:196:A:TYR:H	5	0.23
(1,358)	1:176:A:LEU:HD13	1:196:A:TYR:H	5	0.23
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD11	12	0.23
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD12	12	0.23
(1,335)	1:138:A:ILE:HG21	1:150:A:LEU:HD13	12	0.23
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD11	12	0.23
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD12	12	0.23
(1,335)	1:138:A:ILE:HG22	1:150:A:LEU:HD13	12	0.23
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD11	12	0.23
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD12	12	0.23
(1,335)	1:138:A:ILE:HG23	1:150:A:LEU:HD13	12	0.23
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	14	0.23
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	14	0.23
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	14	0.23
(1,371)	1:192:A:LEU:HD21	1:101:A:LEU:H	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:192:A:LEU:HD22	1:101:A:LEU:H	14	0.22
(1,371)	1:192:A:LEU:HD23	1:101:A:LEU:H	14	0.22
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD11	15	0.22
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD12	15	0.22
(1,348)	1:167:A:LEU:HD11	1:124:A:ILE:HD13	15	0.22
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD11	15	0.22
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD12	15	0.22
(1,348)	1:167:A:LEU:HD12	1:124:A:ILE:HD13	15	0.22
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD11	15	0.22
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD12	15	0.22
(1,348)	1:167:A:LEU:HD13	1:124:A:ILE:HD13	15	0.22
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG11	14	0.22
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG12	14	0.22
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG13	14	0.22
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG11	14	0.22
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG12	14	0.22
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG13	14	0.22
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG11	14	0.22
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG12	14	0.22
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG13	14	0.22
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG21	15	0.21
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG22	15	0.21
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG23	15	0.21
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG21	15	0.21
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG22	15	0.21
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG23	15	0.21
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG21	15	0.21
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG22	15	0.21
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG23	15	0.21
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG21	3	0.21
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG22	3	0.21
(1,370)	1:189:A:LEU:HD11	1:232:A:THR:HG23	3	0.21
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG21	3	0.21
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG22	3	0.21
(1,370)	1:189:A:LEU:HD12	1:232:A:THR:HG23	3	0.21
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG21	3	0.21
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG22	3	0.21
(1,370)	1:189:A:LEU:HD13	1:232:A:THR:HG23	3	0.21
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD11	10	0.21
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD12	10	0.21
(1,341)	1:157:A:LEU:HD11	1:163:A:LEU:HD13	10	0.21
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD11	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD12	10	0.21
(1,341)	1:157:A:LEU:HD12	1:163:A:LEU:HD13	10	0.21
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD11	10	0.21
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD12	10	0.21
(1,341)	1:157:A:LEU:HD13	1:163:A:LEU:HD13	10	0.21
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	2	0.21
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	2	0.21
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	2	0.21
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	11	0.2
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	11	0.2
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	11	0.2
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG11	11	0.2
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG12	11	0.2
(1,336)	1:138:A:ILE:HG21	1:126:A:VAL:HG13	11	0.2
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG11	11	0.2
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG12	11	0.2
(1,336)	1:138:A:ILE:HG22	1:126:A:VAL:HG13	11	0.2
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG11	11	0.2
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG12	11	0.2
(1,336)	1:138:A:ILE:HG23	1:126:A:VAL:HG13	11	0.2
(1,324)	1:101:A:LEU:HD11	1:192:A:LEU:HD11	3	0.19
(1,324)	1:101:A:LEU:HD11	1:192:A:LEU:HD12	3	0.19
(1,324)	1:101:A:LEU:HD11	1:192:A:LEU:HD13	3	0.19
(1,324)	1:101:A:LEU:HD12	1:192:A:LEU:HD11	3	0.19
(1,324)	1:101:A:LEU:HD12	1:192:A:LEU:HD12	3	0.19
(1,324)	1:101:A:LEU:HD12	1:192:A:LEU:HD13	3	0.19
(1,324)	1:101:A:LEU:HD13	1:192:A:LEU:HD11	3	0.19
(1,324)	1:101:A:LEU:HD13	1:192:A:LEU:HD12	3	0.19
(1,324)	1:101:A:LEU:HD13	1:192:A:LEU:HD13	3	0.19
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD21	12	0.19
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD22	12	0.19
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD23	12	0.19
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD21	12	0.19
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD22	12	0.19
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD23	12	0.19
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD21	12	0.19
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD22	12	0.19
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD23	12	0.19
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG21	14	0.18
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG22	14	0.18
(1,399)	1:238:A:LEU:HD21	1:225:A:ILE:HG23	14	0.18
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG21	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG22	14	0.18
(1,399)	1:238:A:LEU:HD22	1:225:A:ILE:HG23	14	0.18
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG21	14	0.18
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG22	14	0.18
(1,399)	1:238:A:LEU:HD23	1:225:A:ILE:HG23	14	0.18
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG21	11	0.18
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG22	11	0.18
(1,330)	1:124:A:ILE:HG21	1:120:A:ILE:HG23	11	0.18
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG21	11	0.18
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG22	11	0.18
(1,330)	1:124:A:ILE:HG22	1:120:A:ILE:HG23	11	0.18
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG21	11	0.18
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG22	11	0.18
(1,330)	1:124:A:ILE:HG23	1:120:A:ILE:HG23	11	0.18
(1,354)	1:173:A:VAL:HG11	1:199:A:ASP:H	2	0.17
(1,354)	1:173:A:VAL:HG12	1:199:A:ASP:H	2	0.17
(1,354)	1:173:A:VAL:HG13	1:199:A:ASP:H	2	0.17
(1,319)	1:89:A:LEU:HD11	1:95:A:ASN:H	8	0.17
(1,319)	1:89:A:LEU:HD12	1:95:A:ASN:H	8	0.17
(1,319)	1:89:A:LEU:HD13	1:95:A:ASN:H	8	0.17
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG21	2	0.16
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG22	2	0.16
(1,343)	1:162:A:THR:HG21	1:207:A:VAL:HG23	2	0.16
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG21	2	0.16
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG22	2	0.16
(1,343)	1:162:A:THR:HG22	1:207:A:VAL:HG23	2	0.16
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG21	2	0.16
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG22	2	0.16
(1,343)	1:162:A:THR:HG23	1:207:A:VAL:HG23	2	0.16
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	14	0.16
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	14	0.16
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	14	0.16
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	14	0.16
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	14	0.16
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	14	0.16
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	14	0.16
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	14	0.16
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	14	0.16
(1,327)	1:120:A:ILE:HD11	1:199:A:ASP:H	7	0.16
(1,327)	1:120:A:ILE:HD12	1:199:A:ASP:H	7	0.16
(1,327)	1:120:A:ILE:HD13	1:199:A:ASP:H	7	0.16
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD21	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD22	13	0.15
(1,323)	1:101:A:LEU:HD11	1:192:A:LEU:HD23	13	0.15
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD21	13	0.15
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD22	13	0.15
(1,323)	1:101:A:LEU:HD12	1:192:A:LEU:HD23	13	0.15
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD21	13	0.15
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD22	13	0.15
(1,323)	1:101:A:LEU:HD13	1:192:A:LEU:HD23	13	0.15
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB1	11	0.15
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB2	11	0.15
(1,318)	1:81:A:VAL:HG11	1:172:A:ALA:HB3	11	0.15
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB1	11	0.15
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB2	11	0.15
(1,318)	1:81:A:VAL:HG12	1:172:A:ALA:HB3	11	0.15
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB1	11	0.15
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB2	11	0.15
(1,318)	1:81:A:VAL:HG13	1:172:A:ALA:HB3	11	0.15
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB1	11	0.15
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB2	11	0.15
(1,318)	1:81:A:VAL:HG21	1:172:A:ALA:HB3	11	0.15
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB1	11	0.15
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB2	11	0.15
(1,318)	1:81:A:VAL:HG22	1:172:A:ALA:HB3	11	0.15
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB1	11	0.15
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB2	11	0.15
(1,318)	1:81:A:VAL:HG23	1:172:A:ALA:HB3	11	0.15
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD11	15	0.14
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD12	15	0.14
(1,389)	1:216:A:THR:HG21	1:205:A:ILE:HD13	15	0.14
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD11	15	0.14
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD12	15	0.14
(1,389)	1:216:A:THR:HG22	1:205:A:ILE:HD13	15	0.14
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD11	15	0.14
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD12	15	0.14
(1,389)	1:216:A:THR:HG23	1:205:A:ILE:HD13	15	0.14
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD11	1	0.14
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD12	1	0.14
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD13	1	0.14
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD11	1	0.14
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD12	1	0.14
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD13	1	0.14
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD11	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD12	1	0.14
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD13	1	0.14
(1,79)	1:113:A:LEU:H	1:115:A:TRP:H	9	0.14
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG21	14	0.13
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG22	14	0.13
(1,350)	1:167:A:LEU:HD21	1:124:A:ILE:HG23	14	0.13
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG21	14	0.13
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG22	14	0.13
(1,350)	1:167:A:LEU:HD22	1:124:A:ILE:HG23	14	0.13
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG21	14	0.13
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG22	14	0.13
(1,350)	1:167:A:LEU:HD23	1:124:A:ILE:HG23	14	0.13
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD21	1	0.13
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD22	1	0.13
(1,338)	1:141:A:LEU:HD21	1:238:A:LEU:HD23	1	0.13
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD21	1	0.13
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD22	1	0.13
(1,338)	1:141:A:LEU:HD22	1:238:A:LEU:HD23	1	0.13
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD21	1	0.13
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD22	1	0.13
(1,338)	1:141:A:LEU:HD23	1:238:A:LEU:HD23	1	0.13
(1,396)	1:237:A:ILE:HD11	1:229:A:CYS:H	12	0.12
(1,396)	1:237:A:ILE:HD12	1:229:A:CYS:H	12	0.12
(1,396)	1:237:A:ILE:HD13	1:229:A:CYS:H	12	0.12
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG21	3	0.12
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG22	3	0.12
(1,384)	1:207:A:VAL:HG11	1:214:A:THR:HG23	3	0.12
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG21	3	0.12
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG22	3	0.12
(1,384)	1:207:A:VAL:HG12	1:214:A:THR:HG23	3	0.12
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG21	3	0.12
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG22	3	0.12
(1,384)	1:207:A:VAL:HG13	1:214:A:THR:HG23	3	0.12
(1,358)	1:176:A:LEU:HD11	1:196:A:TYR:H	13	0.11
(1,358)	1:176:A:LEU:HD12	1:196:A:TYR:H	13	0.11
(1,358)	1:176:A:LEU:HD13	1:196:A:TYR:H	13	0.11
(1,345)	1:163:A:LEU:HD11	1:157:A:LEU:H	7	0.11
(1,345)	1:163:A:LEU:HD12	1:157:A:LEU:H	7	0.11
(1,345)	1:163:A:LEU:HD13	1:157:A:LEU:H	7	0.11
(1,344)	1:163:A:LEU:HD21	1:206:A:LYS:H	14	0.11
(1,344)	1:163:A:LEU:HD22	1:206:A:LYS:H	14	0.11
(1,344)	1:163:A:LEU:HD23	1:206:A:LYS:H	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD11	7	0.11
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD12	7	0.11
(1,334)	1:126:A:VAL:HG21	1:167:A:LEU:HD13	7	0.11
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD11	7	0.11
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD12	7	0.11
(1,334)	1:126:A:VAL:HG22	1:167:A:LEU:HD13	7	0.11
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD11	7	0.11
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD12	7	0.11
(1,334)	1:126:A:VAL:HG23	1:167:A:LEU:HD13	7	0.11
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG21	5	0.1
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG22	5	0.1
(1,333)	1:126:A:VAL:HG21	1:122:A:THR:HG23	5	0.1
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG21	5	0.1
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG22	5	0.1
(1,333)	1:126:A:VAL:HG22	1:122:A:THR:HG23	5	0.1
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG21	5	0.1
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG22	5	0.1
(1,333)	1:126:A:VAL:HG23	1:122:A:THR:HG23	5	0.1

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

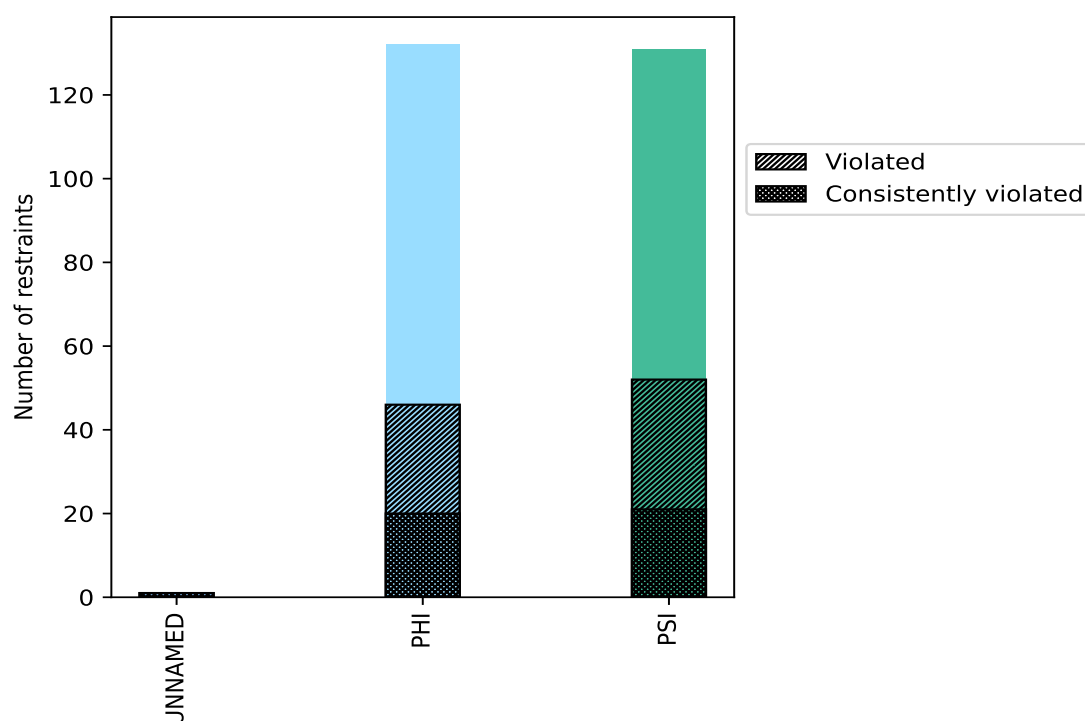
10.1 Summary of dihedral-angle violations [i](#)

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
UNNAMED	1	0.4	1	100.0	0.4	1	100.0	0.4
PHI	132	50.0	46	34.8	17.4	20	15.2	7.6
PSI	131	49.6	52	39.7	19.7	21	16.0	8.0
Total	264	100.0	99	37.5	37.5	42	15.9	15.9

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

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



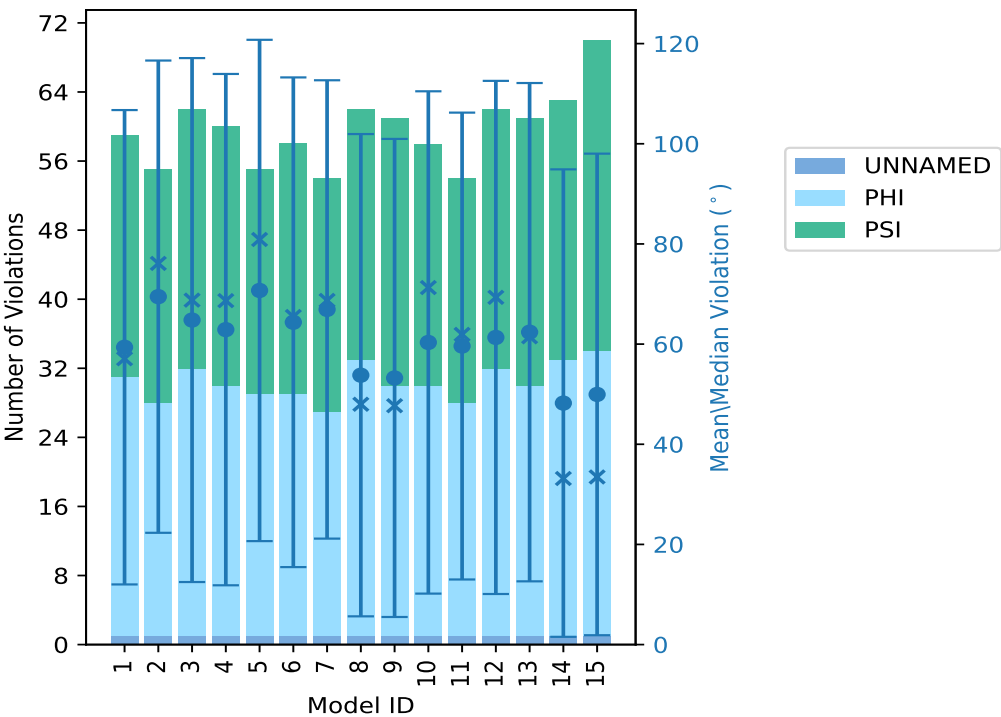
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations				Mean (°)	Max (°)	SD (°)	Median (°)
	UNNAMED	PHI	PSI	Total				
1	1	30	28	59	59.37	157.94	47.36	57.08
2	1	27	27	55	69.47	158.63	47.15	76.11
3	1	31	30	62	64.8	154.25	52.31	68.78
4	1	29	30	60	62.89	159.91	51.05	68.68
5	1	28	26	55	70.71	157.27	50.05	80.89
6	1	28	29	58	64.36	154.67	48.89	65.51
7	1	26	27	54	66.92	156.29	45.76	68.72
8	1	32	29	62	53.79	156.18	48.15	47.99
9	1	29	31	61	53.24	155.36	47.73	47.7
10	1	29	28	58	60.33	154.44	50.15	71.29
11	1	27	26	54	59.61	158.15	46.61	61.94
12	1	31	30	62	61.33	158.65	51.23	69.34
13	1	29	31	61	62.38	155.87	49.75	61.46
14	1	32	30	63	48.22	149.38	46.67	33.16
15	1	33	36	70	49.95	157.54	48.08	33.47

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

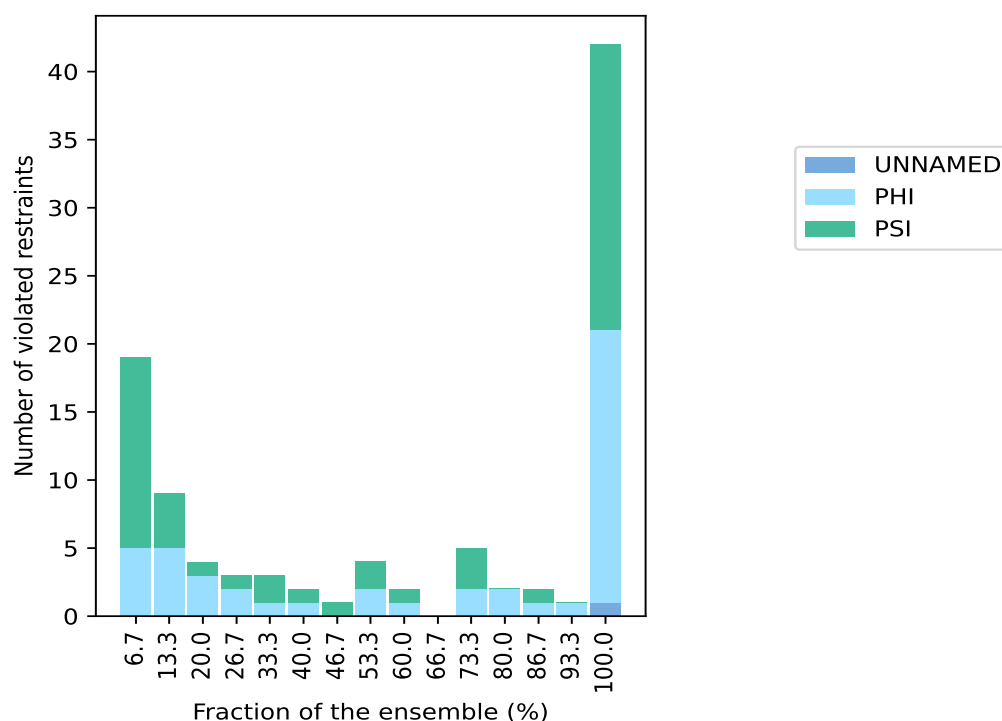
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
UNNAMED	PHI	PSI	Total	Count ¹	%
0	5	14	19	1	6.7
0	5	4	9	2	13.3
0	3	1	4	3	20.0
0	2	1	3	4	26.7
0	1	2	3	5	33.3
0	1	1	2	6	40.0
0	0	1	1	7	46.7
0	2	2	4	8	53.3
0	1	1	2	9	60.0
0	0	0	0	10	66.7
0	2	3	5	11	73.3
0	2	0	2	12	80.0
0	1	1	2	13	86.7
0	1	0	1	14	93.3
1	20	21	42	15	100.0

¹ Number of models with violations

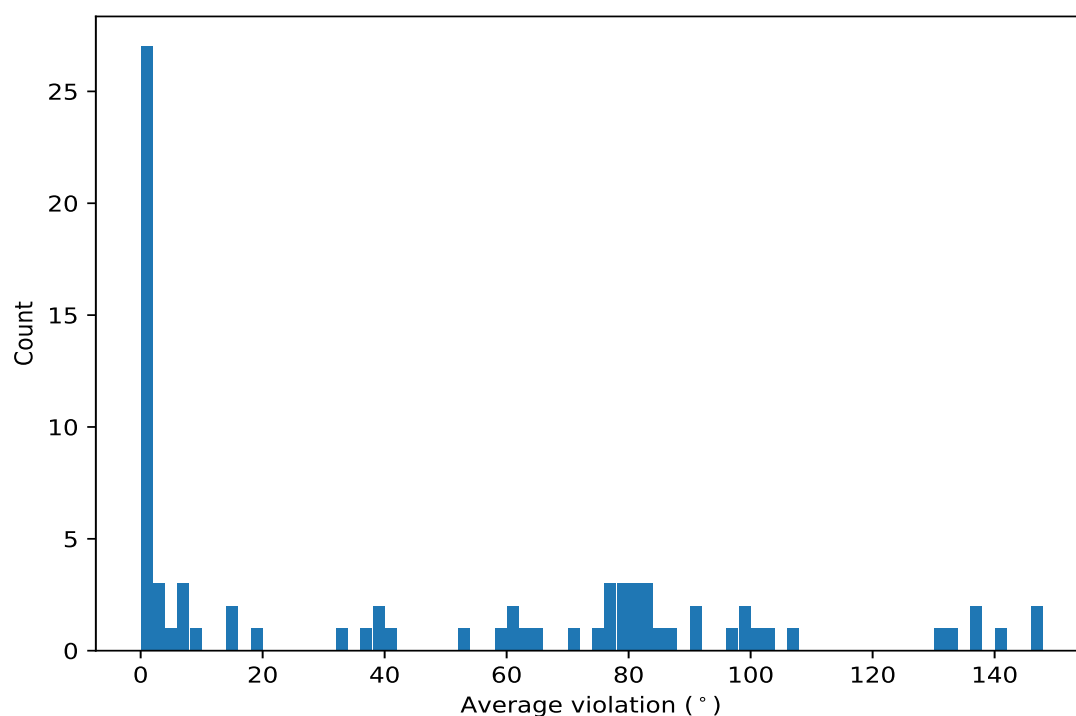
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	15	147.24	7.3	146.93
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	15	146.51	9.14	150.12
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	15	140.87	17.99	145.11
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	15	137.35	8.48	139.51
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	15	136.14	8.36	134.54
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	15	133.15	15.64	130.34
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	15	130.93	19.33	139.44
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	15	106.52	46.81	121.82
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	15	103.28	12.75	105.6
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	15	101.92	10.72	102.33
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	15	98.67	21.03	97.3
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	15	91.67	18.42	99.05
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	15	90.83	5.27	90.31
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	15	87.98	5.5	89.48
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	15	84.47	8.25	83.26
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	15	83.54	15.83	86.29
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	15	82.0	16.54	81.75
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	15	80.88	8.93	82.42
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	15	80.88	10.54	82.48
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	15	78.85	6.83	79.52
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	15	78.32	5.18	77.13

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	15	77.89	7.4	78.16
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	15	77.7	12.54	76.51
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	15	76.77	5.57	76.26
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	15	74.55	52.25	81.68
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	15	71.37	7.34	73.07
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	15	62.1	10.39	61.46
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	15	60.27	12.98	64.02
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	15	60.11	13.01	59.0
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	15	59.06	4.22	58.39
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	15	40.01	34.72	22.83
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	15	38.35	9.38	37.19
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	15	38.12	4.36	38.97
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	15	36.51	6.96	36.74
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	15	33.64	12.28	33.3
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	15	18.48	7.03	18.41
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	15	15.13	6.99	19.0
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	15	14.75	6.28	17.82
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	15	8.66	0.67	8.46
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	15	7.31	3.55	8.61
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	15	4.14	1.61	4.92
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	15	3.66	1.34	4.08
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	14	98.59	45.96	117.18
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	13	96.74	48.85	102.29
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	13	83.45	51.85	112.05
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	12	78.7	47.49	87.22
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	12	1.81	0.6	1.64
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	11	80.9	40.42	88.24
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	11	65.94	49.09	101.32
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	11	52.77	37.04	42.29
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	11	6.97	1.01	7.03
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	11	1.15	0.06	1.16
(1,237)	1:223:A:ASP:C	1:224:A:TYR:N	1:224:A:TYR:CA	1:224:A:TYR:C	9	1.82	0.52	1.56
(1,236)	1:223:A:ASP:N	1:223:A:ASP:CA	1:223:A:ASP:C	1:224:A:TYR:N	9	1.82	0.66	1.5
(1,42)	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1:97:A:VAL:N	8	7.2	4.24	5.92
(1,162)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:LYS:N	8	2.08	0.64	1.9
(1,229)	1:219:A:ARG:C	1:220:A:ASP:N	1:220:A:ASP:CA	1:220:A:ASP:C	8	1.92	0.75	1.84
(1,163)	1:168:A:ILE:C	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	8	1.64	0.23	1.68
(1,228)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:ASP:N	7	1.62	0.5	1.41
(1,192)	1:196:A:TYR:N	1:196:A:TYR:CA	1:196:A:TYR:C	1:197:A:LYS:N	6	1.74	0.74	1.48
(1,189)	1:194:A:LEU:C	1:195:A:VAL:N	1:195:A:VAL:CA	1:195:A:VAL:C	6	1.37	0.33	1.3
(1,233)	1:221:A:VAL:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	5	1.91	0.26	1.81
(1,232)	1:221:A:VAL:N	1:221:A:VAL:CA	1:221:A:VAL:C	1:222:A:VAL:N	5	1.77	0.33	1.58
(1,186)	1:193:A:GLN:N	1:193:A:GLN:CA	1:193:A:GLN:C	1:194:A:LEU:N	5	1.64	0.36	1.75
(1,256)	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	1:239:A:MET:N	4	1.46	0.4	1.32
(1,257)	1:238:A:LEU:C	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	4	1.29	0.12	1.25
(1,195)	1:197:A:LYS:C	1:198:A:PHE:N	1:198:A:PHE:CA	1:198:A:PHE:C	4	1.23	0.16	1.22
(1,247)	1:228:A:LEU:C	1:229:A:CYS:N	1:229:A:CYS:CA	1:229:A:CYS:C	3	1.66	0.45	1.51
(1,246)	1:228:A:LEU:N	1:228:A:LEU:CA	1:228:A:LEU:C	1:229:A:CYS:N	3	1.54	0.38	1.78
(1,161)	1:167:A:LEU:C	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	3	1.45	0.46	1.2
(1,185)	1:192:A:LEU:C	1:193:A:GLN:N	1:193:A:GLN:CA	1:193:A:GLN:C	3	1.37	0.32	1.24
(1,68)	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	1:120:A:ILE:N	2	3.45	0.03	3.45

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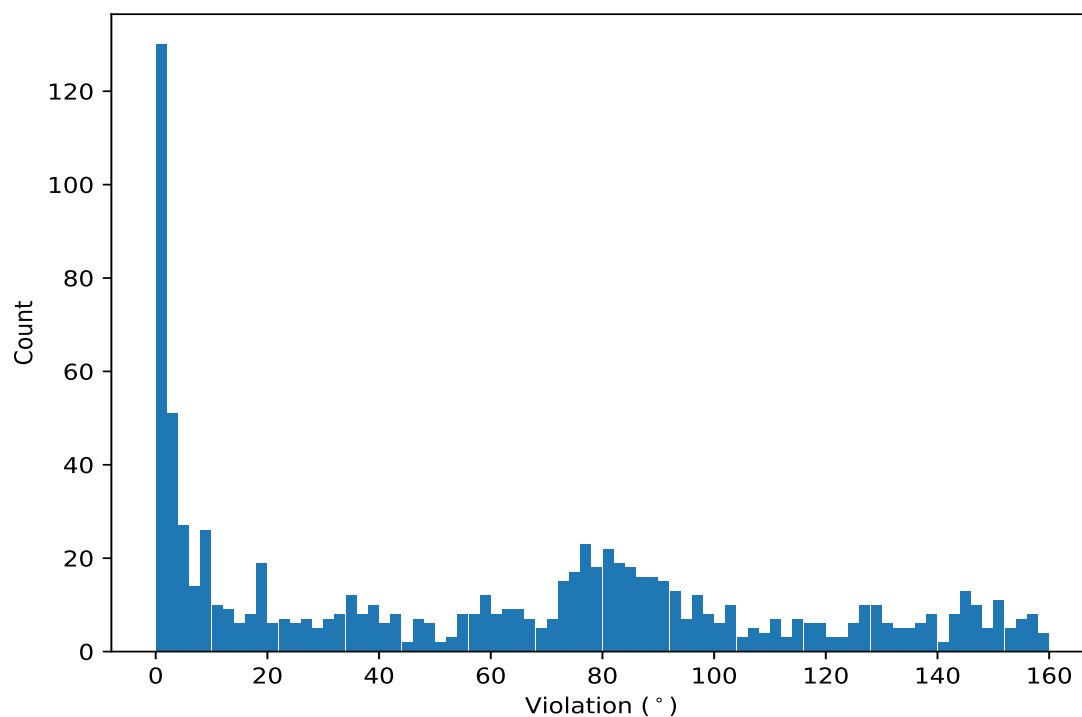
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,12)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:ILE:N	2	1.95	0.26	1.95
(1,205)	1:202:A:GLN:C	1:203:A:ARG:N	1:203:A:ARG:CA	1:203:A:ARG:C	2	1.74	0.69	1.74
(1,188)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:VAL:N	2	1.42	0.15	1.42
(1,191)	1:195:A:VAL:C	1:196:A:TYR:N	1:196:A:TYR:CA	1:196:A:TYR:C	2	1.34	0.04	1.34
(1,187)	1:193:A:GLN:C	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	2	1.23	0.19	1.23
(1,204)	1:202:A:GLN:N	1:202:A:GLN:CA	1:202:A:GLN:C	1:203:A:ARG:N	2	1.23	0.15	1.23
(1,239)	1:224:A:TYR:C	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	2	1.2	0.1	1.2
(1,253)	1:236:A:MET:C	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	2	1.12	0.01	1.12

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 (°)
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	4	159.91
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	12	158.65
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	2	158.63
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	11	158.15
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	1	157.94
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	15	157.54
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	5	157.27
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	12	156.81
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	12	156.7
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	11	156.65
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	7	156.29
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	8	156.18
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	13	155.87
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	11	155.72
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	9	155.36
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	6	154.67
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	10	154.44
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	4	154.39
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	3	154.25
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	9	153.65
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	3	153.17
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	5	152.82
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	10	152.75
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	11	152.06
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	8	151.65
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	3	151.61
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	12	151.47
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	5	151.31
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	8	151.22
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	13	151.02
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	7	150.93
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	2	150.73
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	3	150.19
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	1	150.17
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	6	150.12
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	12	149.94
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	14	149.38
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	6	148.58
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	3	148.47
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	10	148.07
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	4	147.64
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	9	147.32
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	5	147.32
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	12	147.08
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	14	146.93
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	13	146.84
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	4	146.5
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	13	146.29
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	4	146.08
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	15	146.03
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	15	145.95
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	10	145.94

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	5	145.58
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	3	145.4
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	3	145.11
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	13	145.0
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	14	144.91
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	4	144.83
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	4	144.73
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	3	144.57
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	3	144.44
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	5	144.31
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	8	144.12
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	6	143.89
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	13	143.83
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	2	143.61
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	10	143.48
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	9	143.34
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	2	142.92
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	10	142.44
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	13	142.41
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	3	141.03
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	11	140.11
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	1	139.88
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	5	139.51
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	9	139.44
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	6	138.96
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	15	138.78
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	10	138.65
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	6	138.5
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	5	138.43
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	13	137.98
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	9	137.69
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	12	137.13
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	12	136.24
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	2	136.2
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	6	136.07
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	15	135.74
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	7	135.07
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	15	134.54
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	4	134.52
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	7	134.25
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	13	133.32
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1	132.95
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	10	132.94
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	5	132.84
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	5	132.72
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1	131.82
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	8	131.77
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	7	131.73
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1	131.59
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	14	130.37
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	1	130.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	2	129.97
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	9	129.55
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	4	129.2
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	3	128.87
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	15	128.77
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	15	128.42
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	6	128.31
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	4	128.3
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	6	128.28
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	6	128.06
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	7	127.82
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	14	127.68
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	14	127.66
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	8	127.33
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	2	127.29
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	8	127.2
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	11	126.65
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	3	126.65
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	15	126.5
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	2	126.2
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	8	125.99
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	2	125.86
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	15	124.65
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	7	124.61
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	1	124.38
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	11	124.0
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	2	123.83
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	10	123.39
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	7	122.7
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	10	121.82
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	14	121.01
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	3	120.87
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	15	119.69
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	1	119.41
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	7	119.24
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	7	118.52
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	2	118.52
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	7	118.3
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	15	117.61
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	4	116.61
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	13	116.57
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	6	116.52
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	12	116.46
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	13	116.46
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	6	115.98
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	12	115.91
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	1	115.87
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	13	115.05
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	2	114.64
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	6	114.54
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	2	114.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	12	113.6
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	6	113.5
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	5	112.05
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	4	111.99
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	8	111.67
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	5	111.27
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	5	110.89
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	12	110.42
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	2	110.38
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	11	110.13
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	7	109.83
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	2	109.82
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	9	109.53
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	3	108.52
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	8	107.81
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	7	107.74
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	10	107.04
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	5	106.99
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	2	106.13
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	7	105.81
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	3	105.6
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	4	104.8
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	3	103.74
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	9	103.71
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	13	103.49
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	11	103.3
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	9	103.22
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	7	102.89
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	14	102.34
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	8	102.33
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	11	102.29
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	5	102.24
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	12	101.99
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	4	101.58
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	4	101.32
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	12	101.15
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	14	100.61
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	2	100.31
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	15	99.73
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	1	99.67
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	4	99.12
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	3	99.05
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	6	98.77
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	13	98.24
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	12	98.2
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	1	98.1
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	14	97.99
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	3	97.89
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	7	97.83
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	13	97.83
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	13	97.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	7	97.48
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	1	97.3
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	5	97.06
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	6	96.92
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	10	96.83
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	12	96.73
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	12	96.7
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	5	95.89
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1	95.43
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	9	94.84
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	11	94.77
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	10	94.72
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	1	94.65
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	14	94.35
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	8	93.9
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	3	93.72
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	12	93.55
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	4	93.54
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	14	93.44
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	13	92.94
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	5	92.9
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	7	92.78
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	15	92.61
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	2	92.39
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	9	92.37
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	3	92.36
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	6	92.05
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	2	91.97
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	8	91.89
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	5	91.8
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	4	91.62
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	14	91.49
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	3	91.35
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	11	91.21
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	5	91.1
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	13	90.81
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	4	90.78
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	5	90.47
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	1	90.4
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	4	90.36
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	9	90.31
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	11	90.3
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	2	89.84
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	1	89.69
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	6	89.66
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	9	89.65
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	12	89.48
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	8	89.06
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	4	89.0
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	7	88.82
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	6	88.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	7	88.64
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	8	88.47
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1	88.47
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	9	88.39
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	10	88.31
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	12	88.24
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	12	88.14
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	13	87.9
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	12	87.48
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	13	87.36
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	9	87.3
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	5	87.28
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	10	87.18
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	9	86.68
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	2	86.62
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	6	86.62
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	2	86.51
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	8	86.4
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1	86.35
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	11	86.32
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	11	86.29
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	8	86.28
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	4	86.13
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	1	85.98
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	14	85.79
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	13	85.77
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	8	85.33
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	10	85.24
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	6	85.16
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	6	85.14
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	5	84.95
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	13	84.93
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	13	84.82
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	1	84.78
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	3	84.77
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	14	84.58
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	8	84.35
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	3	84.18
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	12	84.15
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	2	84.07
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	1	84.03
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	7	83.51
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	15	83.4
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	5	83.37
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	14	83.26
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	5	83.25
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	10	83.25
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	12	83.08
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	14	83.07
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	12	82.99
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	5	82.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	10	82.74
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	7	82.48
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	9	82.47
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	10	82.42
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	12	82.42
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	4	82.2
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	9	82.19
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	1	82.18
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	11	82.16
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	9	81.88
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	15	81.82
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	14	81.75
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	5	81.68
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	10	81.67
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	10	81.54
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	2	81.52
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	10	81.28
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	4	81.23
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	5	80.89
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	12	80.86
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	4	80.82
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	6	80.63
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	15	80.6
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	11	80.59
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	3	80.59
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	13	80.53
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	8	80.39
(1,176)	1:180:A:GLN:C	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	14	80.24
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	10	80.21
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	15	80.16
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	9	80.0
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	13	79.68
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	11	79.65
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	2	79.52
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	9	79.43
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1	79.42
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	5	79.31
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	5	79.03
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	5	78.99
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	6	78.88
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	3	78.72
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	11	78.45
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	9	78.35
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	9	78.35
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	7	78.3
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	13	78.16
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	10	78.07
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	2	78.05
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	7	78.03
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	1	77.87
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	14	77.78

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	15	77.77
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	3	77.56
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	3	77.55
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	11	77.43
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	10	77.37
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	6	77.27
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	6	77.13
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	12	77.09
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	8	77.08
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	15	77.03
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	8	76.99
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	14	76.96
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	13	76.96
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	11	76.81
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	8	76.79
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	2	76.67
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	15	76.51
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	10	76.34
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	1	76.32
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	15	76.26
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	2	76.11
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	7	75.17
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	7	75.17
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	14	75.11
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	4	74.91
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	8	74.82
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	11	74.74
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	14	74.71
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	13	74.6
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	8	74.53
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	10	74.34
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	4	74.2
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	14	74.2
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	15	74.18
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	8	74.16
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	12	74.13
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	10	74.13
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	12	74.03
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	10	73.71
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	2	73.68
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	6	73.59
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	4	73.46
(1,173)	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1:178:A:SER:N	15	73.43
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	15	73.41
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	13	73.25
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	12	73.07
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	14	73.05
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	11	72.65
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	4	72.37
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	15	72.35
(1,172)	1:177:A:VAL:C	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	3	72.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	5	72.17
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	2	72.11
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	3	71.75
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	6	71.56
(1,178)	1:181:A:PRO:C	1:182:A:ILE:N	1:182:A:ILE:CA	1:182:A:ILE:C	7	71.41
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	3	71.2
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	1	70.94
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	11	70.26
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	11	70.03
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	4	69.66
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	3	69.05
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	10	68.87
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	8	68.52
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	3	68.51
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	4	67.69
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	3	67.65
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	6	67.13
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	13	66.84
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	5	66.28
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	9	66.11
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	7	66.02
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	11	65.72
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	12	65.61
(1,168)	1:175:A:LYS:C	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	10	65.18
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	15	65.14
(1,171)	1:176:A:LEU:N	1:176:A:LEU:CA	1:176:A:LEU:C	1:177:A:VAL:N	7	65.02
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	5	64.84
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	15	64.8
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	1	64.26
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	11	64.02
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	6	63.89
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	7	63.54
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	15	63.51
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	14	63.41
(1,174)	1:178:A:SER:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	3	62.86
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	14	62.71
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	9	62.4
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	7	62.18
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	14	62.07
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	10	61.79
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	13	61.46
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	8	61.29
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	12	60.76
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	8	60.7
(1,169)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LEU:N	2	60.43
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	10	60.21
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	15	60.09
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	2	59.99
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	6	59.93
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	11	59.87
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	9	59.81

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	9	59.15
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	11	59.1
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	4	59.03
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	1	59.01
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	2	59.0
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	14	58.74
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	12	58.39
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	8	58.2
(1,240)	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	1:259:A:ALA:N	11	57.87
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	10	57.52
(1,175)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	4	57.18
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	1	57.08
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	13	56.7
(1,112)	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1:180:A:GLN:N	1	56.11
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	7	56.1
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	6	56.04
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	8	55.93
(1,84)	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	1:128:A:THR:N	2	55.68
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	1	55.2
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	2	55.0
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	4	54.35
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	9	54.26
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	13	54.25
(1,43)	1:129:A:SER:C	1:97:A:VAL:N	1:97:A:VAL:CA	1:97:A:VAL:C	3	54.05
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	7	53.68
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	13	53.36
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	7	53.19
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	1	51.93
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	13	51.6
(1,170)	1:176:A:LEU:C	1:177:A:VAL:N	1:177:A:VAL:CA	1:177:A:VAL:C	9	49.39
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	15	49.37
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1	49.16
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	13	48.73
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	6	48.54
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	4	48.03
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	9	47.7
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	3	47.66
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	5	46.72
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	5	46.34
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	9	46.29
(1,177)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:181:A:PRO:N	1	46.15
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	6	46.08
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	5	45.93
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	9	45.76
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	5	43.87
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	4	43.76
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	4	43.2
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	14	43.0
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	1	42.99
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	2	42.35
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1	42.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	15	42.29
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	13	41.98
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	13	41.86
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	3	41.33
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	11	40.84
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	11	40.61
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	8	40.05
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	12	39.95
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	5	39.83
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	3	39.81
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	6	39.33
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	10	38.97
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	10	38.87
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	11	38.83
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	4	38.17
(1,179)	1:181:A:PRO:N	1:181:A:PRO:CA	1:181:A:PRO:C	1:182:A:ILE:N	6	38.07
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	12	38.04
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	7	37.85
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	10	37.77
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	7	37.25
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	2	37.19
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	13	37.18
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	9	36.84
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	6	36.74
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	12	36.47
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	15	35.77
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	2	35.71
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	6	35.69
(1,201)	1:233:A:THR:C	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	15	35.54
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	12	35.23
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	8	35.11
(1,217)	1:246:A:LYS:C	1:214:A:THR:N	1:214:A:THR:CA	1:214:A:THR:C	15	35.09
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	8	34.81
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	2	34.49
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	11	34.18
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	3	34.1
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	6	34.08
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	2	33.52
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	8	33.3
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	14	33.24
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	11	33.17
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	14	33.16
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	8	32.8
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1	32.79
(1,110)	1:145:A:TRP:N	1:145:A:TRP:CA	1:145:A:TRP:C	1:179:A:VAL:N	6	32.06
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	15	31.85
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	7	31.14
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	8	31.01
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	8	30.71
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	15	30.57
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	7	30.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,113)	1:179:A:VAL:C	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	11	30.28
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	3	29.24
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	7	29.21
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	14	28.64
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	15	28.13
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	3	28.03
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	8	27.83
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	12	27.6
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	13	27.06
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	13	26.61
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	5	26.35
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	12	26.33
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	14	26.01
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	7	25.11
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	2	24.76
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	8	24.75
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	14	24.52
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	9	24.08
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	15	24.06
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	15	23.83
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	15	23.65
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	6	23.14
(1,34)	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	1:91:A:THR:N	11	23.1
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	7	22.83
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	7	22.75
(1,241)	1:225:A:ILE:C	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	14	22.04
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	5	21.34
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	11	21.12
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	4	20.42
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	3	20.18
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	9	20.12
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	6	20.08
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	7	19.75
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	11	19.73
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	15	19.68
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	10	19.47
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	2	19.42
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	9	19.38
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1	19.34
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	6	19.3
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	12	19.0
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	11	18.99
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	2	18.94
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	7	18.88
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	1	18.84
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	8	18.8
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	15	18.73
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	13	18.65
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	4	18.64
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	14	18.41
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	3	18.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,167)	1:174:A:PRO:N	1:174:A:PRO:CA	1:174:A:PRO:C	1:175:A:LYS:N	14	17.96
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	4	17.82
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	11	17.81
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	12	17.77
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	13	17.58
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	15	17.45
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	3	17.44
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	3	17.09
(1,264)	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	1:243:A:PHE:N	9	15.57
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	2	14.97
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	12	14.41
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	9	14.38
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	9	14.34
(1,42)	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1:97:A:VAL:N	10	14.08
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	1	13.98
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	4	13.89
(1,180)	1:182:A:ILE:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	1	13.25
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	5	12.89
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	6	12.51
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	9	12.36
(1,263)	1:241:A:SER:C	1:275:A:LEU:N	1:275:A:LEU:CA	1:275:A:LEU:C	13	12.33
(1,42)	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1:97:A:VAL:N	6	12.33
(1,262)	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1:275:A:LEU:N	4	12.27
(1,208)	1:204:A:LEU:N	1:204:A:LEU:CA	1:204:A:LEU:C	1:205:A:ILE:N	15	11.51
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	11	11.26
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	9	11.21
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	2	11.16
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	5	11.14
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	9	11.07
(1,111)	1:145:A:TRP:C	1:179:A:VAL:N	1:179:A:VAL:CA	1:179:A:VAL:C	2	10.61
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	7	10.56
(1,42)	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1:97:A:VAL:N	14	10.17
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	1	10.09
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	9	9.96
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	6	9.9
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	11	9.65
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	13	9.48
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	15	9.18
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	2	8.83
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	2	8.72
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	4	8.61
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	14	8.57
(1,243)	1:259:A:ALA:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	15	8.54
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	15	8.53
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	3	8.49
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	6	8.48
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	10	8.47
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	12	8.47
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	4	8.46
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	8	8.46
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	13	8.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	1	8.44
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	9	8.44
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	11	8.42
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	14	8.41
(1,130)	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1:155:A:ARG:N	7	8.35
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	12	8.21
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	13	8.09
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	7	8.01
(1,209)	1:204:A:LEU:C	1:205:A:ILE:N	1:205:A:ILE:CA	1:205:A:ILE:C	15	7.92
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	1	7.76
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	9	7.73
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	3	7.71
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	1	7.58
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	6	7.44
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	12	7.18
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	11	7.03
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	1	6.99
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	15	6.65
(1,42)	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1:97:A:VAL:N	3	6.59
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	9	6.53
(1,69)	1:152:A:ALA:C	1:120:A:ILE:N	1:120:A:ILE:CA	1:120:A:ILE:C	10	6.41
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	4	6.35
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	12	5.98
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	13	5.85
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	9	5.68
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	12	5.65
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	12	5.6
(1,260)	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	1:241:A:SER:N	3	5.52
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	15	5.39
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	10	5.26
(1,42)	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1:97:A:VAL:N	13	5.26
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	6	5.24
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	2	5.13
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	13	5.04
(1,83)	1:126:A:VAL:C	1:160:A:ASN:N	1:160:A:ASN:CA	1:160:A:ASN:C	2	5.03
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	1	5.02
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	3	4.92
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	15	4.81
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	6	4.79
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	8	4.73
(1,42)	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1:97:A:VAL:N	4	4.62
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	7	4.44
(1,190)	1:195:A:VAL:N	1:195:A:VAL:CA	1:195:A:VAL:C	1:196:A:TYR:N	9	4.4
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	3	4.3
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	10	4.25
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	2	4.23
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	13	4.19
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	1	4.08
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	14	4.04
(1,202)	1:201:A:LYS:N	1:201:A:LYS:CA	1:201:A:LYS:C	1:202:A:GLN:N	15	3.98
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	7	3.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	4	3.8
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	5	3.63
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	11	3.59
(1,258)	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	1:240:A:GLY:N	5	3.58
(1,229)	1:219:A:ARG:C	1:220:A:ASP:N	1:220:A:ASP:CA	1:220:A:ASP:C	15	3.57
(1,68)	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	1:120:A:ILE:N	9	3.48
(1,68)	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	1:120:A:ILE:N	14	3.42
(1,42)	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1:97:A:VAL:N	7	3.31
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	15	3.3
(1,192)	1:196:A:TYR:N	1:196:A:TYR:CA	1:196:A:TYR:C	1:197:A:LYS:N	15	3.28
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	8	3.23
(1,259)	1:239:A:MET:C	1:240:A:GLY:N	1:240:A:GLY:CA	1:240:A:GLY:C	14	3.16
(1,236)	1:223:A:ASP:N	1:223:A:ASP:CA	1:223:A:ASP:C	1:224:A:TYR:N	4	3.15
(1,237)	1:223:A:ASP:C	1:224:A:TYR:N	1:224:A:TYR:CA	1:224:A:TYR:C	4	3.13
(1,162)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:LYS:N	15	3.08
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	4	3.0
(1,162)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:LYS:N	6	2.99
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	11	2.91
(1,206)	1:203:A:ARG:N	1:203:A:ARG:CA	1:203:A:ARG:C	1:204:A:LEU:N	15	2.74
(1,228)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:ASP:N	15	2.71
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	5	2.65
(1,224)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:ASP:N	15	2.62
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	10	2.56
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	5	2.55
(1,236)	1:223:A:ASP:N	1:223:A:ASP:CA	1:223:A:ASP:C	1:224:A:TYR:N	3	2.51
(1,205)	1:202:A:GLN:C	1:203:A:ARG:N	1:203:A:ARG:CA	1:203:A:ARG:C	15	2.43
(1,199)	1:199:A:ASP:C	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1	2.41
(1,232)	1:221:A:VAL:N	1:221:A:VAL:CA	1:221:A:VAL:C	1:222:A:VAL:N	4	2.4
(1,236)	1:223:A:ASP:N	1:223:A:ASP:CA	1:223:A:ASP:C	1:224:A:TYR:N	13	2.36
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	9	2.32
(1,162)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:LYS:N	13	2.32
(1,233)	1:221:A:VAL:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	4	2.31
(1,247)	1:228:A:LEU:C	1:229:A:CYS:N	1:229:A:CYS:CA	1:229:A:CYS:C	14	2.27
(1,229)	1:219:A:ARG:C	1:220:A:ASP:N	1:220:A:ASP:CA	1:220:A:ASP:C	14	2.24
(1,12)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:ILE:N	4	2.21
(1,229)	1:219:A:ARG:C	1:220:A:ASP:N	1:220:A:ASP:CA	1:220:A:ASP:C	6	2.2
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	5	2.19
(1,237)	1:223:A:ASP:C	1:224:A:TYR:N	1:224:A:TYR:CA	1:224:A:TYR:C	3	2.16
(1,256)	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	1:239:A:MET:N	8	2.14
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	5	2.14
(1,233)	1:221:A:VAL:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	3	2.1
(1,161)	1:167:A:LEU:C	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	9	2.1
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	8	2.08
(1,186)	1:193:A:GLN:N	1:193:A:GLN:CA	1:193:A:GLN:C	1:194:A:LEU:N	4	2.06
(1,200)	1:233:A:THR:N	1:233:A:THR:CA	1:233:A:THR:C	1:201:A:LYS:N	11	2.04
(1,162)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:LYS:N	8	2.03
(1,108)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:TRP:N	13	2.01
(1,229)	1:219:A:ARG:C	1:220:A:ASP:N	1:220:A:ASP:CA	1:220:A:ASP:C	3	2.0
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	2	2.0
(1,163)	1:168:A:ILE:C	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	6	1.95
(1,189)	1:194:A:LEU:C	1:195:A:VAL:N	1:195:A:VAL:CA	1:195:A:VAL:C	3	1.94

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,237)	1:223:A:ASP:C	1:224:A:TYR:N	1:224:A:TYR:CA	1:224:A:TYR:C	13	1.92
(1,210)	1:205:A:ILE:N	1:205:A:ILE:CA	1:205:A:ILE:C	1:206:A:LYS:N	15	1.9
(1,186)	1:193:A:GLN:N	1:193:A:GLN:CA	1:193:A:GLN:C	1:194:A:LEU:N	14	1.87
(1,192)	1:196:A:TYR:N	1:196:A:TYR:CA	1:196:A:TYR:C	1:197:A:LYS:N	2	1.86
(1,163)	1:168:A:ILE:C	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	13	1.86
(1,246)	1:228:A:LEU:N	1:228:A:LEU:CA	1:228:A:LEU:C	1:229:A:CYS:N	10	1.83
(1,233)	1:221:A:VAL:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	14	1.81
(1,163)	1:168:A:ILE:C	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	10	1.81
(1,185)	1:192:A:LEU:C	1:193:A:GLN:N	1:193:A:GLN:CA	1:193:A:GLN:C	8	1.8
(1,232)	1:221:A:VAL:N	1:221:A:VAL:CA	1:221:A:VAL:C	1:222:A:VAL:N	3	1.79
(1,163)	1:168:A:ILE:C	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	15	1.79
(1,246)	1:228:A:LEU:N	1:228:A:LEU:CA	1:228:A:LEU:C	1:229:A:CYS:N	14	1.78
(1,162)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:LYS:N	10	1.76
(1,186)	1:193:A:GLN:N	1:193:A:GLN:CA	1:193:A:GLN:C	1:194:A:LEU:N	8	1.75
(1,162)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:LYS:N	2	1.75
(1,236)	1:223:A:ASP:N	1:223:A:ASP:CA	1:223:A:ASP:C	1:224:A:TYR:N	12	1.74
(1,228)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:ASP:N	3	1.74
(1,228)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:ASP:N	6	1.74
(1,233)	1:221:A:VAL:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	12	1.73
(1,134)	1:252:A:PRO:N	1:252:A:PRO:CA	1:252:A:PRO:C	1:253:A:LYS:N	15	1.73
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	11	1.72
(1,12)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:ILE:N	12	1.69
(1,237)	1:223:A:ASP:C	1:224:A:TYR:N	1:224:A:TYR:CA	1:224:A:TYR:C	5	1.68
(1,229)	1:219:A:ARG:C	1:220:A:ASP:N	1:220:A:ASP:CA	1:220:A:ASP:C	13	1.68
(1,192)	1:196:A:TYR:N	1:196:A:TYR:CA	1:196:A:TYR:C	1:197:A:LYS:N	5	1.66
(1,233)	1:221:A:VAL:C	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	1	1.6
(1,189)	1:194:A:LEU:C	1:195:A:VAL:N	1:195:A:VAL:CA	1:195:A:VAL:C	12	1.6
(1,232)	1:221:A:VAL:N	1:221:A:VAL:CA	1:221:A:VAL:C	1:222:A:VAL:N	14	1.58
(1,162)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:LYS:N	9	1.58
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	10	1.57
(1,163)	1:168:A:ILE:C	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	8	1.57
(1,237)	1:223:A:ASP:C	1:224:A:TYR:N	1:224:A:TYR:CA	1:224:A:TYR:C	9	1.56
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	6	1.56
(1,188)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:VAL:N	3	1.56
(1,237)	1:223:A:ASP:C	1:224:A:TYR:N	1:224:A:TYR:CA	1:224:A:TYR:C	1	1.55
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	7	1.55
(1,232)	1:221:A:VAL:N	1:221:A:VAL:CA	1:221:A:VAL:C	1:222:A:VAL:N	1	1.54
(1,232)	1:221:A:VAL:N	1:221:A:VAL:CA	1:221:A:VAL:C	1:222:A:VAL:N	12	1.54
(1,237)	1:223:A:ASP:C	1:224:A:TYR:N	1:224:A:TYR:CA	1:224:A:TYR:C	10	1.53
(1,247)	1:228:A:LEU:C	1:229:A:CYS:N	1:229:A:CYS:CA	1:229:A:CYS:C	10	1.51
(1,186)	1:193:A:GLN:N	1:193:A:GLN:CA	1:193:A:GLN:C	1:194:A:LEU:N	15	1.51
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	14	1.5
(1,236)	1:223:A:ASP:N	1:223:A:ASP:CA	1:223:A:ASP:C	1:224:A:TYR:N	1	1.5
(1,257)	1:238:A:LEU:C	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	8	1.49
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	8	1.49
(1,236)	1:223:A:ASP:N	1:223:A:ASP:CA	1:223:A:ASP:C	1:224:A:TYR:N	9	1.49
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	10	1.47
(1,237)	1:223:A:ASP:C	1:224:A:TYR:N	1:224:A:TYR:CA	1:224:A:TYR:C	12	1.47
(1,229)	1:219:A:ARG:C	1:220:A:ASP:N	1:220:A:ASP:CA	1:220:A:ASP:C	4	1.46
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	3	1.46
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	4	1.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,195)	1:197:A:LYS:C	1:198:A:PHE:N	1:198:A:PHE:CA	1:198:A:PHE:C	1	1.45
(1,187)	1:193:A:GLN:C	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	4	1.42
(1,228)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:ASP:N	13	1.41
(1,189)	1:194:A:LEU:C	1:195:A:VAL:N	1:195:A:VAL:CA	1:195:A:VAL:C	8	1.41
(1,163)	1:168:A:ILE:C	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	11	1.4
(1,237)	1:223:A:ASP:C	1:224:A:TYR:N	1:224:A:TYR:CA	1:224:A:TYR:C	14	1.39
(1,228)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:ASP:N	4	1.39
(1,191)	1:195:A:VAL:C	1:196:A:TYR:N	1:196:A:TYR:CA	1:196:A:TYR:C	8	1.38
(1,163)	1:168:A:ILE:C	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	2	1.38
(1,256)	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	1:239:A:MET:N	14	1.37
(1,204)	1:202:A:GLN:N	1:202:A:GLN:CA	1:202:A:GLN:C	1:203:A:ARG:N	15	1.37
(1,196)	1:198:A:PHE:N	1:198:A:PHE:CA	1:198:A:PHE:C	1:199:A:ASP:N	8	1.37
(1,255)	1:237:A:ILE:C	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	8	1.36
(1,203)	1:201:A:LYS:C	1:202:A:GLN:N	1:202:A:GLN:CA	1:202:A:GLN:C	13	1.34
(1,195)	1:197:A:LYS:C	1:198:A:PHE:N	1:198:A:PHE:CA	1:198:A:PHE:C	8	1.33
(1,163)	1:168:A:ILE:C	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	14	1.33
(1,228)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:ASP:N	14	1.32
(1,239)	1:224:A:TYR:C	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	15	1.3
(1,194)	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	1:198:A:PHE:N	9	1.3
(1,191)	1:195:A:VAL:C	1:196:A:TYR:N	1:196:A:TYR:CA	1:196:A:TYR:C	1	1.3
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	14	1.29
(1,192)	1:196:A:TYR:N	1:196:A:TYR:CA	1:196:A:TYR:C	1:197:A:LYS:N	11	1.29
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	11	1.29
(1,192)	1:196:A:TYR:N	1:196:A:TYR:CA	1:196:A:TYR:C	1:197:A:LYS:N	7	1.27
(1,188)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:VAL:N	12	1.27
(1,257)	1:238:A:LEU:C	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	14	1.26
(1,256)	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	1:239:A:MET:N	10	1.26
(1,160)	1:167:A:LEU:N	1:167:A:LEU:CA	1:167:A:LEU:C	1:168:A:ILE:N	9	1.26
(1,42)	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	1:97:A:VAL:N	11	1.25
(1,257)	1:238:A:LEU:C	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	12	1.24
(1,185)	1:192:A:LEU:C	1:193:A:GLN:N	1:193:A:GLN:CA	1:193:A:GLN:C	15	1.24
(1,254)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:LEU:N	14	1.23
(1,236)	1:223:A:ASP:N	1:223:A:ASP:CA	1:223:A:ASP:C	1:224:A:TYR:N	5	1.23
(1,261)	1:240:A:GLY:C	1:241:A:SER:N	1:241:A:SER:CA	1:241:A:SER:C	8	1.22
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	6	1.21
(1,250)	1:230:A:ASP:N	1:230:A:ASP:CA	1:230:A:ASP:C	1:231:A:ALA:N	8	1.2
(1,247)	1:228:A:LEU:C	1:229:A:CYS:N	1:229:A:CYS:CA	1:229:A:CYS:C	8	1.2
(1,236)	1:223:A:ASP:N	1:223:A:ASP:CA	1:223:A:ASP:C	1:224:A:TYR:N	10	1.2
(1,229)	1:219:A:ARG:C	1:220:A:ASP:N	1:220:A:ASP:CA	1:220:A:ASP:C	1	1.2
(1,189)	1:194:A:LEU:C	1:195:A:VAL:N	1:195:A:VAL:CA	1:195:A:VAL:C	5	1.2
(1,161)	1:167:A:LEU:C	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	12	1.2
(1,197)	1:198:A:PHE:C	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	9	1.19
(1,183)	1:191:A:HIS:C	1:192:A:LEU:N	1:192:A:LEU:CA	1:192:A:LEU:C	8	1.18
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	13	1.18
(1,236)	1:223:A:ASP:N	1:223:A:ASP:CA	1:223:A:ASP:C	1:224:A:TYR:N	14	1.17
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	1	1.17
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	9	1.17
(1,257)	1:238:A:LEU:C	1:239:A:MET:N	1:239:A:MET:CA	1:239:A:MET:C	9	1.16
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	4	1.16
(1,253)	1:236:A:MET:C	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	12	1.13
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	15	1.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,253)	1:236:A:MET:C	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	14	1.11
(1,195)	1:197:A:LYS:C	1:198:A:PHE:N	1:198:A:PHE:CA	1:198:A:PHE:C	3	1.11
(1,162)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:LYS:N	14	1.11
(1,239)	1:224:A:TYR:C	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	11	1.1
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	10	1.1
(1,256)	1:238:A:LEU:N	1:238:A:LEU:CA	1:238:A:LEU:C	1:239:A:MET:N	5	1.09
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	7	1.09
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	12	1.09
(1,204)	1:202:A:GLN:N	1:202:A:GLN:CA	1:202:A:GLN:C	1:203:A:ARG:N	10	1.08
(1,60)	1:113:A:LEU:N	1:113:A:LEU:CA	1:113:A:LEU:C	1:114:A:LEU:N	9	1.07
(1,10)	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:C	1:79:A:LEU:N	12	1.07
(1,228)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:ASP:N	1	1.06
(1,189)	1:194:A:LEU:C	1:195:A:VAL:N	1:195:A:VAL:CA	1:195:A:VAL:C	15	1.06
(1,185)	1:192:A:LEU:C	1:193:A:GLN:N	1:193:A:GLN:CA	1:193:A:GLN:C	7	1.06
(1,205)	1:202:A:GLN:C	1:203:A:ARG:N	1:203:A:ARG:CA	1:203:A:ARG:C	10	1.05
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	10	1.05
(1,192)	1:196:A:TYR:N	1:196:A:TYR:CA	1:196:A:TYR:C	1:197:A:LYS:N	6	1.05
(1,161)	1:167:A:LEU:C	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	3	1.05
(1,129)	1:155:A:ARG:C	1:156:A:GLN:N	1:156:A:GLN:CA	1:156:A:GLN:C	14	1.05
(1,229)	1:219:A:ARG:C	1:220:A:ASP:N	1:220:A:ASP:CA	1:220:A:ASP:C	10	1.04
(1,195)	1:197:A:LYS:C	1:198:A:PHE:N	1:198:A:PHE:CA	1:198:A:PHE:C	14	1.04
(1,187)	1:193:A:GLN:C	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	5	1.04
(1,193)	1:196:A:TYR:C	1:197:A:LYS:N	1:197:A:LYS:CA	1:197:A:LYS:C	12	1.02
(1,186)	1:193:A:GLN:N	1:193:A:GLN:CA	1:193:A:GLN:C	1:194:A:LEU:N	13	1.01
(1,246)	1:228:A:LEU:N	1:228:A:LEU:CA	1:228:A:LEU:C	1:229:A:CYS:N	8	1.0
(1,189)	1:194:A:LEU:C	1:195:A:VAL:N	1:195:A:VAL:CA	1:195:A:VAL:C	6	1.0